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Prediction of Mineral Quality of Irrigation Return Flow. Volume III. Simulation Model of Conjunctive Use and Water Quality for a River System or Basin

Bureau of Reclamation, Denver, Colo. Engineering & Research Ctr.

Prepared for

Robert S. Kerr Environmental Research Lab, Ada, Okla.

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The development and evaluation of modeling capability to simulate and predict the effects of irrigation on the quality of return flows are documented in the five volumes of this report. The report contains two different modeling packages which represent different levels of detail and sophistication. Volumes I, II, and IV pertain to the model package given in Volume III. Volume V contains the more sophisticated model. User's manuals are included in Volumes III and V.

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PREDICTION OF MINERAL QUALITY OF IRRIGATION RETURN FLOW

VOLUME III

SIMULATION MODEL OF CONJUNCTIVE USE AND WATER QUALITY FOR A RIVER SYSTEM OR BASIN

USER'S MANUAL

by

Bureau of Reclamation
Engineering and Research Center
Denver, Colorado 80225

EPA-IAG-D4-0371

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FOREWORD

The Environmental Protection Agency was established to coordinate administration of the major Federal programs designed to protect the quality of our environment.

An important part of the Agency's effort involves the search for information about environmental problems, management techniques and new technologies through which optimum use of the Nation's land and water resources can be assured and the threat pollution poses to the welfare of the American people can be minimized.

EPA's Office of Research and Development conducts this search through a nationwide network of research facilities.

As one of these facilities, the Robert S. Kerr Environmental Research Laboratory is responsible for the management of programs to: (a) investigate the nature, transport, fate and management of pollutants in groundwater; (b) develop and demonstrate methods for treating wastewaters with soil and other natural systems; (c) develop and demonstrate pollution control technologies for irrigation return flows; (d) develop and demonstrate pollution control technologies for animal production wastes; (e) develop and demonstrate technologies to prevent, control or abate pollution from the petroleum refining and petrochemical industries; and (f) develop and demonstrate technologies to manage pollution resulting from combinations of industrial wastewaters or industrial/municipal wastewaters.

This report contributes to the knowledge essential if the EPA is to meet the requirements of environmental laws that it establish and enforce pollution control standards which are reasonable, cost effective and provide adequate protection for the American public.

William C Galegar

William C. Galegar
Director
Robert S. Kerr Environmental
Research Laboratory

PREFACE

This report is one of a set which documents the development and verification of a digital computer modeling effort to predict the mineral quality changes in return flows occurring as a result of irrigating agricultural lands. The set consists of five separate volumes under one general title as follows:

"Prediction of Mineral Quality of Irrigation Return Flow"

Volume I.	Summary Report and Verification
Volume II.	Vernal Field Study
Volume III.	Simulation Model of Conjunctive Use and Water Quality for a River Basin System
Volume IV.	Data Analysis Utility Programs
Volume V.	Detailed Return Flow Salinity and Nutrient Simulation Model

This set of reports represents the culmination of an effort started in May 1969 by an interagency agreement between the U.S. Bureau of Reclamation and the Federal Water Pollution Control Administration on a joint research proposal on the "Prediction of Mineral Quality of Return Flow Water from Irrigated Land." This research project has had three different project identification numbers during the project period. These numbers (13030 EII, EPA-IAG-048-(D), and EPA-IAG-D4-0371) are given to avoid confusion on the part of individuals who have previously tried to acquire project reports for the earlier project numbers.

ABSTRACT

This volume of the report documents the development of a digital computer coded simulation model to predict the effect of irrigation of agricultural lands on the resulting irrigation return flow quality. The model is capable of simulating conjunctive uses of water, however, validation for this purpose was not performed. The model developed in this volume is much less rigorous than that presented in Volume V, however, it can be used to provide an assessment of water quality trends due to irrigation at much less cost than the detailed model. A user's manual is included in the report.

This report was submitted in fulfillment of EPA-IAG-D4-0371 by the Bureau of Reclamation, Engineering and Research Center, under the sponsorship of the Environmental Protection Agency.

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INTRODUCTION

The majority of present day analyses or studies of river basin water resources are made for the purpose of increasing certain yields of an existing physical system or to determine the critical attributes of an undesirable salinity profile.

The size and complexity of nearly all river basin studies prohibit the use of manual efforts in obtaining solutions to the multitude of variations of the physical system operation. Consequently, such river basin studies are mathematically modeled as electronic computer applications.

A number of mathematical models are available for use in studying the physical systems of a river basin. Linear and nonlinear programing techniques are the basis for some of these models and yet others are simulation models with varying degrees of complexity and flexibility.

The availability of so many models makes it quite apparent that a generalized model that would encompass all the objectives in studying a river basin is an impossible task.

In the early stages of the conceptual design of this mathematical model it was realized that limitations due to the varying objectives, model flexibility, and electronic computer capabilities were going to be major factors in setting the design framework for the model.

A primary concern in the design of this model was the provision of maximum flexibility. An examination of other models indicated that most analysts and managers were interested in obtaining physically feasible solutions. A physically feasible solution is defined as the operation of a river basin physical system with a given set of criteria and/or constraints such that the desired objective could be accomplished if the system is simulated with this defined format for "X" number of years in the future. The flexibility then becomes important because several objectives might be included in the study of a river basin, and certainly no two river basins are identical.

This examination also revealed a great interest in not only studying the hydrology but also the changes in salinity within a given river basin. These changes are often referred to as "salt loading."

Subsequent to the collection of model requirements and the perspective gained in the aforementioned examination, it was concluded that an overall model should be designed as two separate submodels; namely, a data analysis submodel and a simulation submodel.

The data analysis submodel as well as the simulation submodel are complete and operational at this time.

In this volume the simulation submodel will be discussed in detail and another volume will contain the description of the data analysis submodel.

THE CONJUNCTIVE USE SIMULATION MODEL

The conjunctive use capabilities of the model are those required to simulate simultaneously the use of water resources within the river basin from both surface resources and subsurface or ground-water resources.

These capabilities include the resource magnitude as well as its chemical quality. The chemical quality of the water resource is further characterized in terms of eight inorganic constituents as well as the total salts.

The overall simulation model has as a basis a nodal concept or structure which facilitates the mathematical representation of a river basin and a simple compact manner of performing calculations, many of which are iterative in design.

A river basin can be studied as one node or as many as 20 nodes. The model is designed for a maximum of 20 nodes; however, this maximum is determined by the limitations of the computer system being used. The number of nodes used in a particular river basin study will be a decision the analyst must make on the basis of data available, the number of response points desired, and the physical features within the river basin. The node then as a common denominator can be used to represent the simplest river basin study to one that is quite complex.

The node can include the simulation of one or all of the following features:

a. Ten tributary inflows

b. Ten demands of water resources, both surface and subsurface

c. The operation of a surface reservoir

d. The operation of a power facility

e. The operation of a subsurface reservoir (aquifer)

f. The percolation of surface waters vertically through a soil column

g. The operation of a pumping facility

h. The determination of return flows, both magnitude and quality, when given consumptive use and conveyance losses.

A pictorial representation of the node features is shown on Figure 1 . An example of a river basin with three nodes is shown on Figure 2. The symbolic box representation of the three nodes and the symbolic representation of the operation sequence of one node are shown on Figures 3 and 4 , respectively.

The electronic computer application of the conjunctive use simulation model consists of 24 subroutines or functions plus the executive or main program. The FORTRAN listings included as part of this volume for the main program as well as the subroutines and functions are filled with comments at pertinent points. The extensive use of these comments is meant to aid in describing the flow of the model and to provide information within the listings that would be helpful in making program modifications or conversions to other computer systems as either become necessary.

The general flow of the model as controlled by the main or executive program (ACUMEN) is shown on Figure 5. Many different formats have been used in the presentation of a user's manual. The format used in this volume will contain one-page flow charts with the aid of extensive narrative which should provide ease of reading and yet be as comprehensive as possible.

A list of variable names and arrays and usages thereof will be inserted at the end of each program, subroutine, or function description. A majority of variable names and data arrays used in the model will be contained within several labeled common blocks.

NODE FEATURES

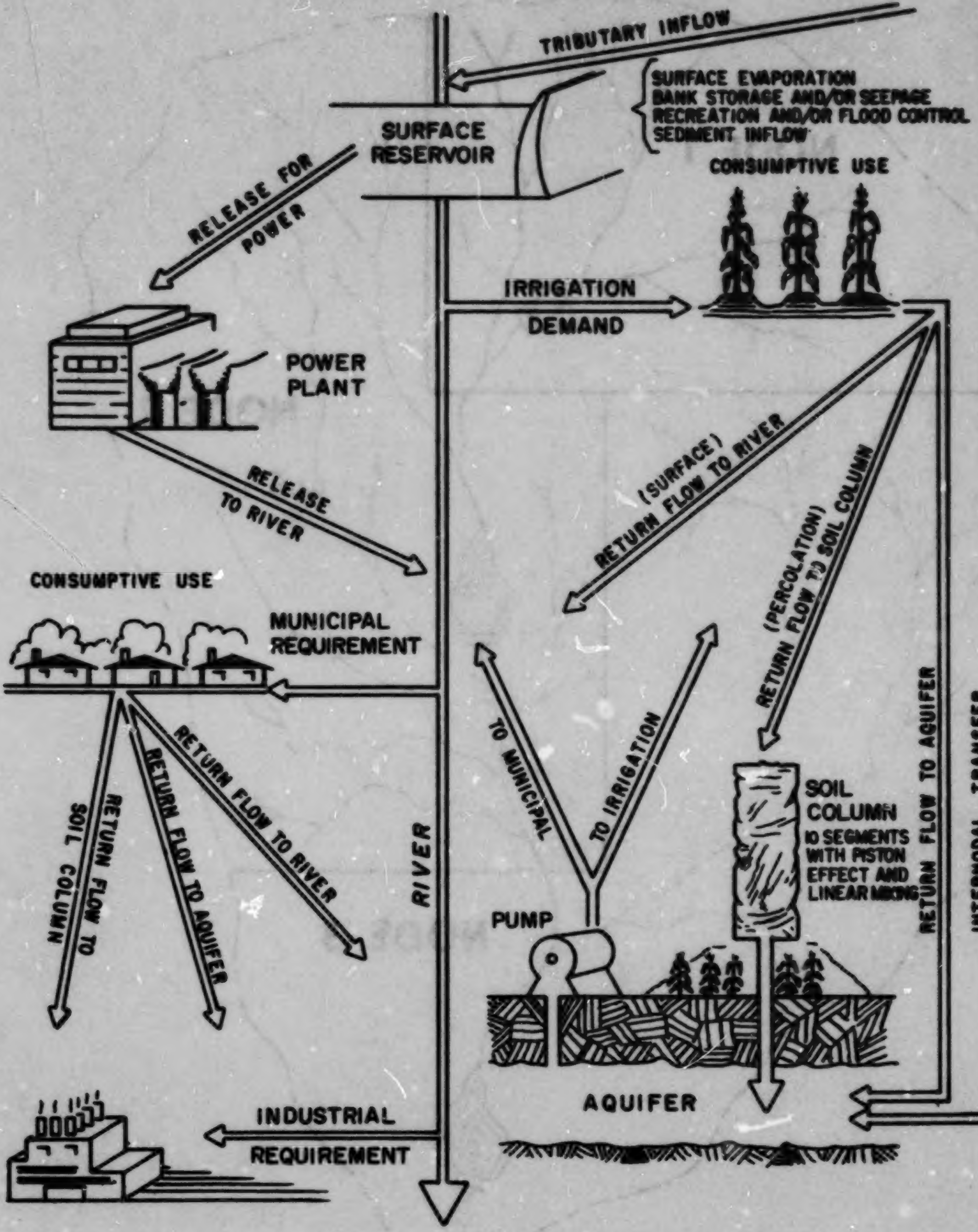

TRIBUTARY INFLOW
SURFACE EVAPORATION
BANK STORAGE AND/OR SEEPAGE
RECREATION AND/OR FLOOD CONTROL
SEDIMENT INFLOW
SURFACE RESERVOIR
CONSUMPTIVE USE
RELEASE FOR POWER
IRRIGATION
DEMAND
POWER PLANT
RELEASE TO RIVER
(SURFACE) RETURN FLOW TO RIVER
(PERCOLATION) RETURN FLOW TO SOIL COLUMN
CONSUMPTIVE USE
MUNICIPAL REQUIREMENT
TO MUNICIPAL
TO IRRIGATION
RETURN FLOW TO AQUIFER
INTERNODAL TRANSFER
RETURN FLOW TO SOIL COLUMN
RETURN FLOW TO AQUIFER
RETURN FLOW TO RIVER
RIVER
SOIL COLUMN
10 SEGMENTS WITH PISTON EFFECT AND LINEAR MIXING
PUMP
AQUIFER
INDUSTRIAL
REQUIREMENT

FIGURE 1

16

EXAMPLE RIVER BASIN

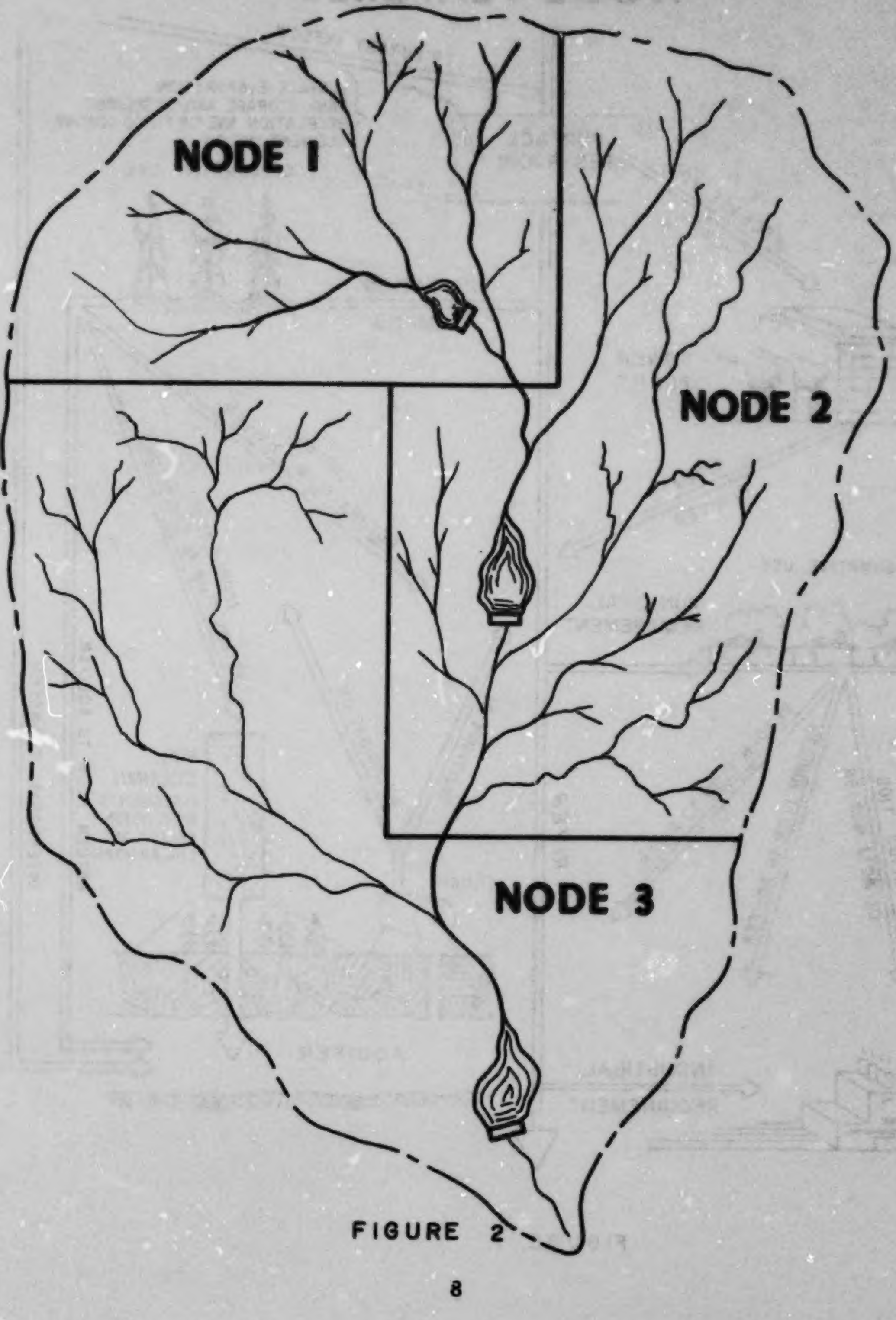

NODE 1
NODE 2
NODE 3

FIGURE 2

SYMBOLIC NODE STRUCTURE OF RIVER BASIN

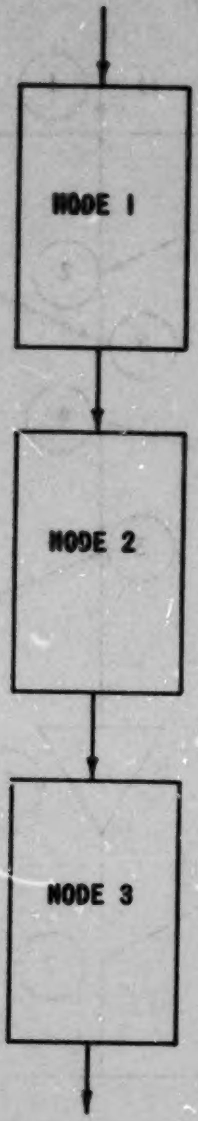
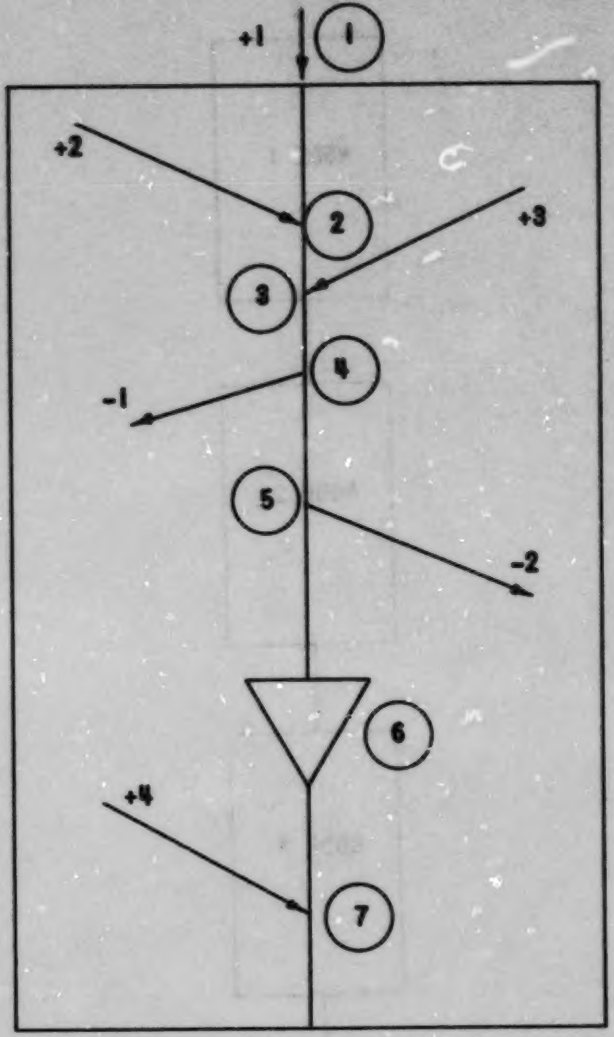

NODE 1
NODE 2
NODE 3

FIGURE 3

EXAMPLE
NODE WITH SEVEN OPERATION SEQUENCES



+1
1
+2
2
+3
3
4
-1
5
-2
6
+4
7

+ = Inflow
- = Demands

FIGURE 4

GENERAL FLOW OF MODEL

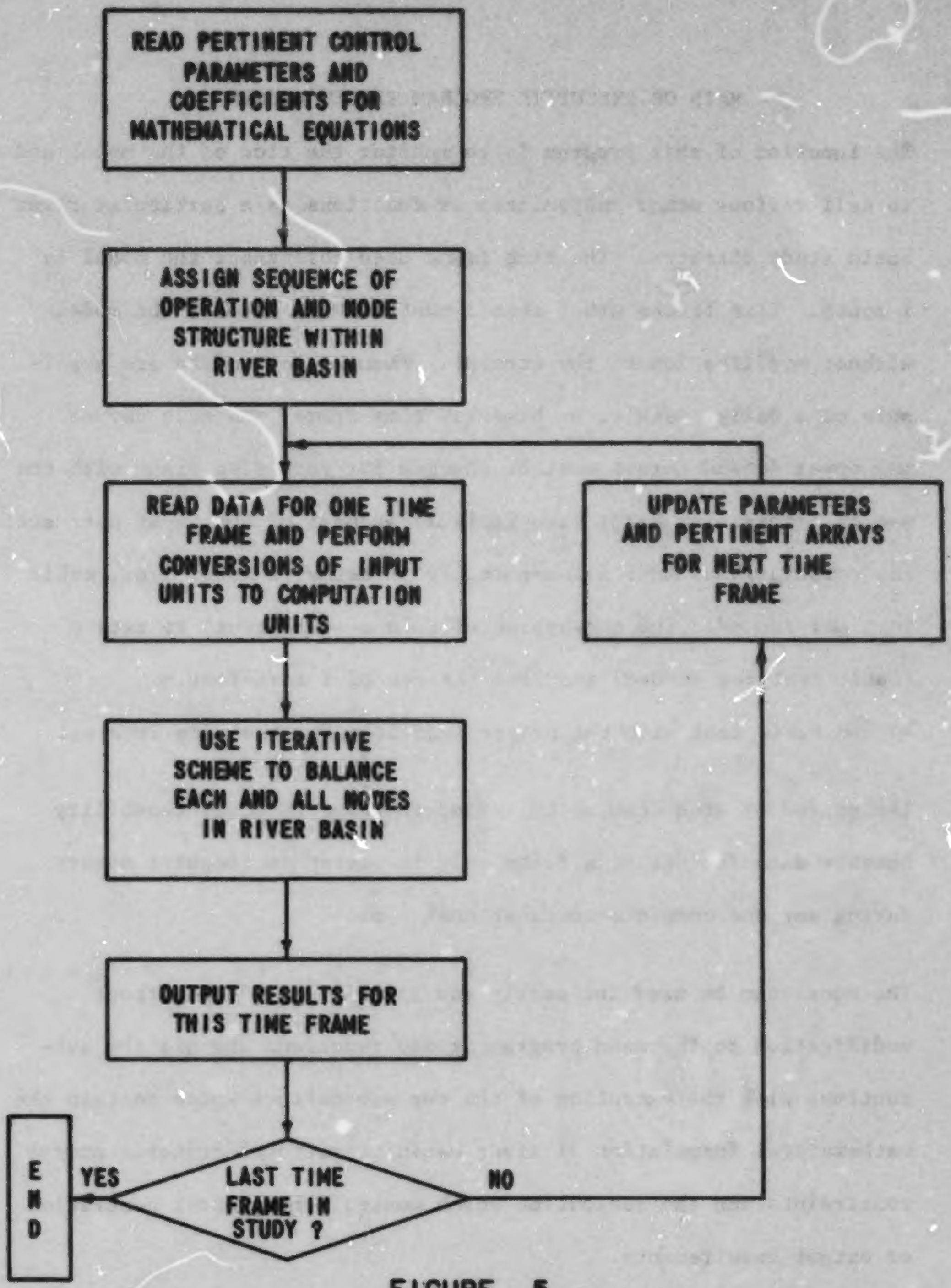

READ PERTINENT CONTROL PARAMETERS AND COEFFICIENTS FOR MATHEMATICAL EQUATIONS
ASSIGN SEQUENCE OF OPERATION AND NODE STRUCTURE WITHIN RIVER BASIN
READ DATA FOR ONE TIME FRAME AND PERFORM CONVERSIONS OF INPUT UNITS TO COMPUTATION UNITS
UPDATE PARAMETERS AND PERTINENT ARRAYS FOR NEXT TIME FRAME
USE ITERATIVE SCHEME TO BALANCE EACH AND ALL NODES IN RIVER BASIN
OUTPUT RESULTS FOR THIS TIME FRAME
LAST TIME FRAME IN STUDY ?
YES
NO
END

FIGURE 5

MAIN OR EXECUTIVE PROGRAM TITLED ACUMEN

The function of this program is to monitor the flow of the model and to call various other subroutines or functions as a particular river basin study dictates. The time frame used throughout the model is 1 month. Time frames other than 1 month can be used in the model without modification to the concept. When historic data are available on a daily, weekly, or biweekly time frame, the rule curves and power demand curves must be changed for each time frame with the use of transaction cards (see Table 2) as part of the input data set. The computational mode is essentially in terms of rate; i.e., cubic feet per second. The conversion of volume (acre-feet) to rate (cubic feet per second) requires the use of 1 acre-foot = 43,560 cubic feet with the proper transform for the time interval.

The period of study can be unlimited in terms of model capability because data for one time frame only is stored in computer memory during any one complete computational cycle.

The model can be used for nearly any river basin study without modification to the main program or the functions and all the subroutines with the exception of the two subroutines which contain the mathematical formulation of river basin operational criteria and/or constraints and the subroutine which controls the report generation or output requirements.

The model will accept input data on punched cards or data on magnetic tape. The input unit is assigned a variable name in the main program and can be changed to fit the physical form of the input data. The model requires 42,000 words of rapid access memory.

An earlier version of the simulation model contained a subroutine titled "CONTRL" which has been discarded in favor of a set of control cards read in as input and the related logic placed in the main program. The control cards and logic allow the manipulation of the data set (as did the subroutine CONTRL) without the usual redistribution of the data set to accommodate an alternate study whereby certain physical features of a river basin are omitted or added as required.

The complete comprehension and appreciation of this capability can only be acquired through the application of the model to more than one river basin study.

General flow charts, as shown on Figures 6 to 12, indicate how demands, inflows, subsurface to surface transfers, surface to subsurface transfers, subsurface to subsurface transfers (internodal), surface reservoirs, and subsurface reservoirs (aquifers) are treated in the iterative scheme.

The iterative scheme begins with the node farthest upstream in the river basin and completes the hydrologic balance along with the chemistry mixes in that node and continues downstream to the next node and completes the hydrologic balance and chemistry mixes using both nodes and in this manner proceeds to the most downstream node, and therefore the whole river basin is balanced.

Whenever a node cannot be balanced hydrologically or a shortage exceeds the preset shortage index, an appropriate error message will be printed and computation will be terminated.

Each time a surface reservoir in an upstream node makes a release to meet a deficit in a downstream demand, the iterative scheme begins again at that point and updates the flow and chemistry of the river, which updates the chemistry of all downstream demands as they are affected by the upstream reservoir release. The reiteration through the basin from point of incremental surface supply to the point of deficit is made to update all chemistry with respect to constraining salinity levels for demands and for selective withdrawals from both surface and subsurface storage facilities.

The simulation of waters percolating vertically through a soil column is the last operation completed in each node balance. The requirement of the soil column simulation is determined by inspection of the volume of water stored in TTANK which acts symbolically as a ponding pool on the surface for waters to be percolated.

The use of surface to subsurface and subsurface to surface transfers is an excellent mechanism for a "black box" approach to return flow lag times and excess surface flows that cannot be expressed explicitly because of inadequate data.

The report generating routines are called from the main program as well as the routines containing the operational criteria. As mentioned earlier in this volume, these routines must be designed anew for each specific river basin to be studied.

The variable names or data arrays used in the main program are shown in Table 1.

ITERATIVE SCHEME-GENERAL

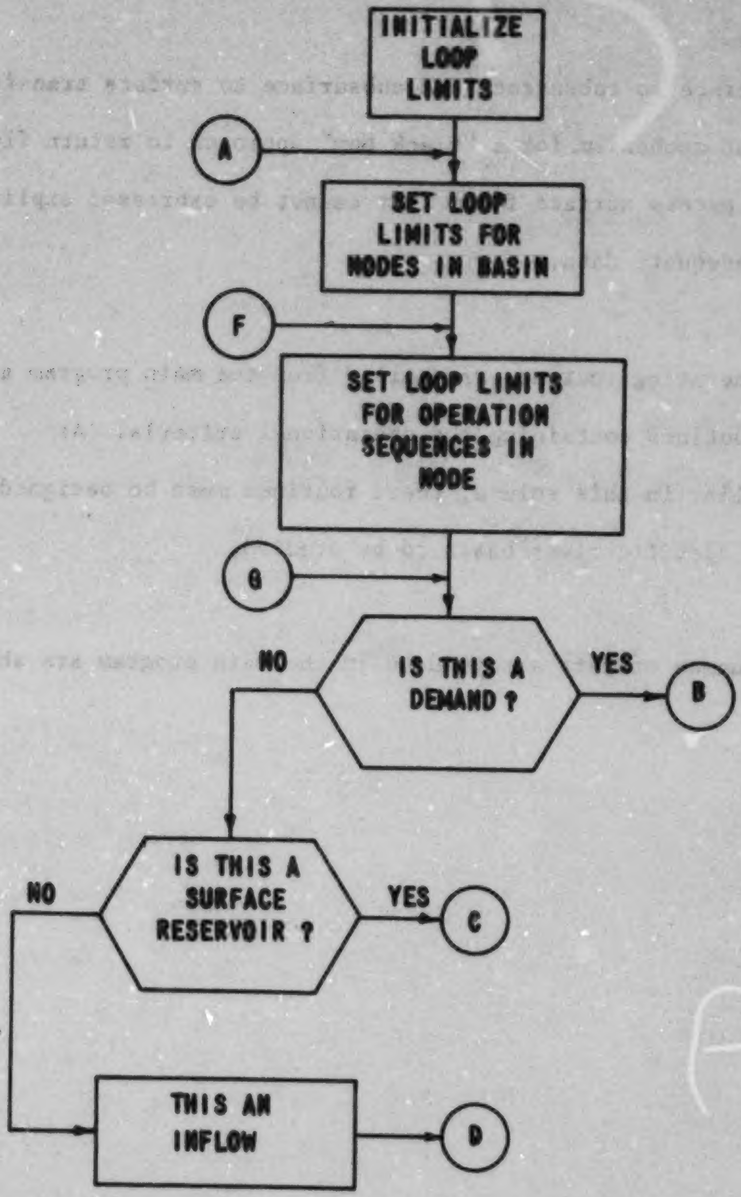

INITIALIZE LOOP LIMITS
A
SET LOOP LIMITS FOR NODES IN BASIN
F
SET LOOP LIMITS FOR OPERATION SEQUENCES IN NODE
G
IS THIS A DEMAND ?
NO
YES
B
IS THIS A SURFACE RESERVOIR ?
NO
YES
C
THIS AN INFLOW
D

FIGURE 6

ITERATIVE SCHEME-DEMANDS

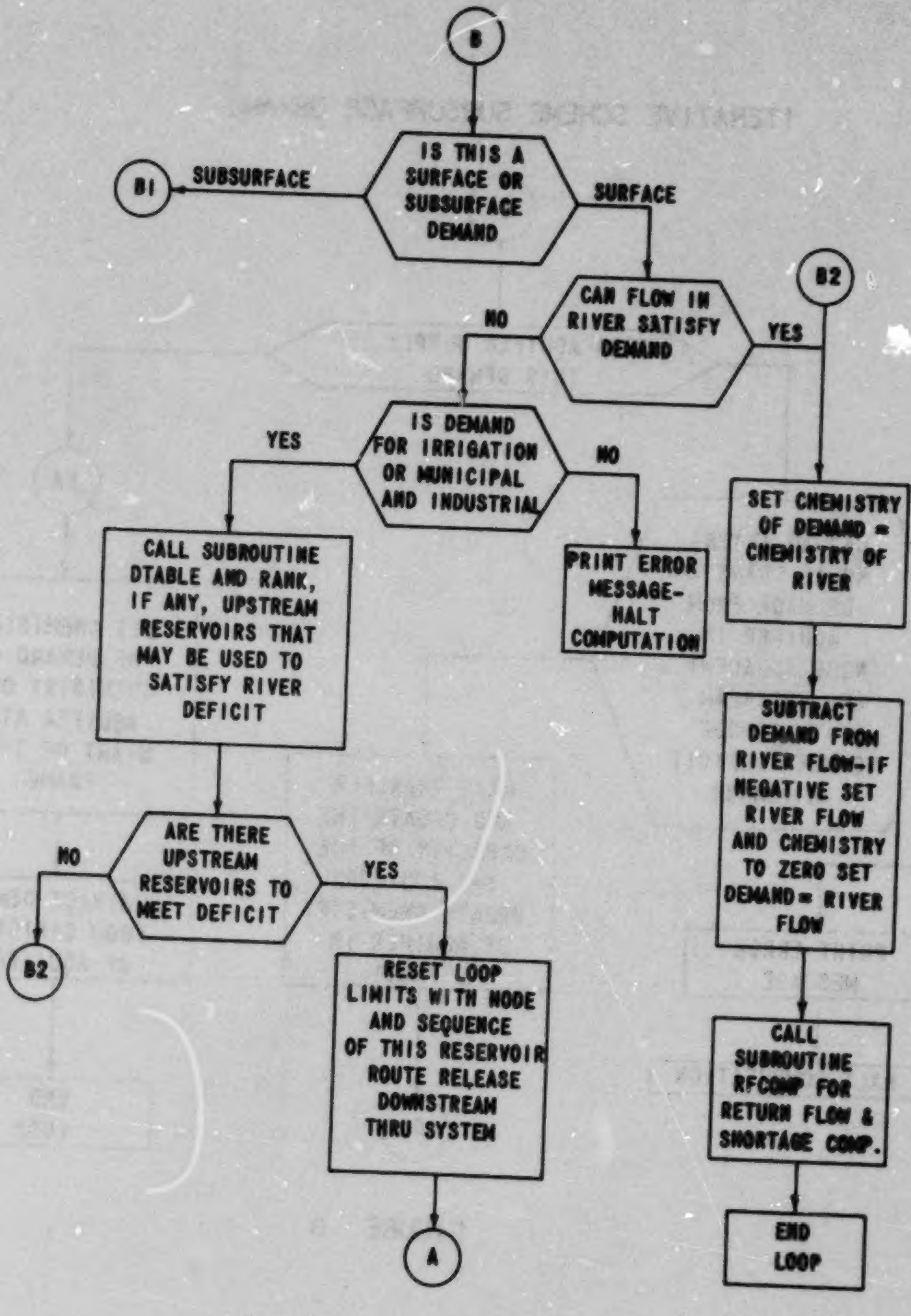

B
IS THIS A SURFACE OR SUBSURFACE DEMAND
SUBSURFACE
B1
SURFACE
CAN FLOW IN RIVER SATISFY DEMAND
NO
YES
B2
IS DEMAND FOR IRRIGATION OR MUNICIPAL AND INDUSTRIAL
YES
NO
CALL SUBROUTINE DTABLE AND RANK, IF ANY, UPSTREAM RESERVOIRS THAT MAY BE USED TO SATISFY RIVER DEFICIT
PRINT ERROR MESSAGE-HALT COMPUTATION
SET CHEMISTRY OF DEMAND = CHEMISTRY OF RIVER
SUBTRACT DEMAND FROM RIVER FLOW-IF NEGATIVE SET RIVER FLOW AND CHEMISTRY TO ZERO SET DEMAND = RIVER FLOW
ARE THERE UPSTREAM RESERVOIRS TO MEET DEFICIT
NO
YES
B2
RESET LOOP LIMITS WITH NODE AND SEQUENCE OF THIS RESERVOIR ROUTE RELEASE DOWNSTREAM THRU SYSTEM
CALL SUBROUTINE RFCOMP FOR RETURN FLOW & SHORTAGE COMP.
END LOOP
A

FIGURE 7

ITERATIVE SCHEME-SUBSURFACE DEMAND

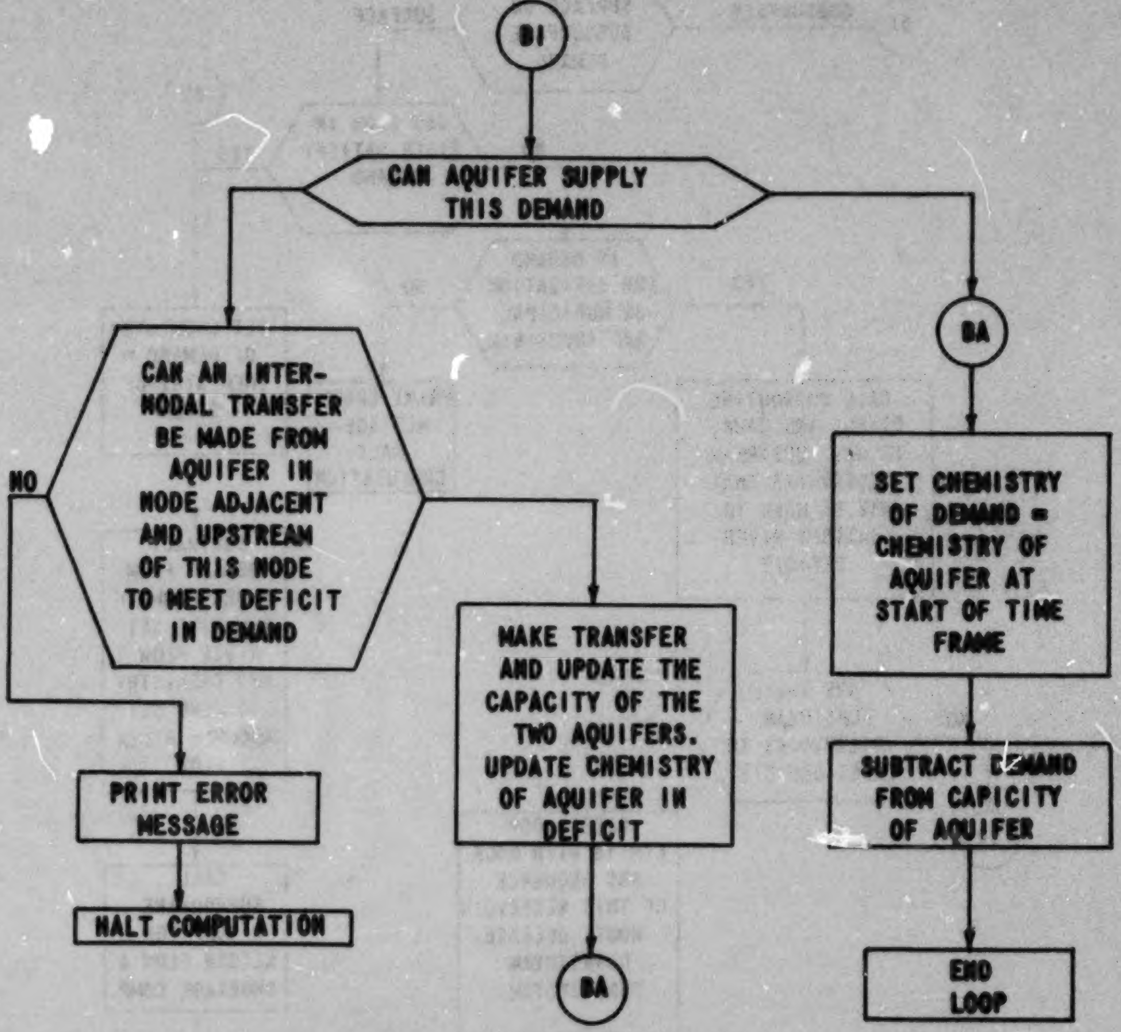

BI
CAN AQUIFER SUPPLY THIS DEMAND
CAN AN INTER-NODAL TRANSFER BE MADE FROM AQUIFER IN NODE ADJACENT AND UPSTREAM OF THIS NODE TO MEET DEFICIT IN DEMAND
NO
PRINT ERROR MESSAGE
HALT COMPUTATION
MAKE TRANSFER AND UPDATE THE CAPACITY OF THE TWO AQUIFERS. UPDATE CHEMISTRY OF AQUIFER IN DEFICIT
BA
BA
SET CHEMISTRY OF DEMAND = CHEMISTRY OF AQUIFER AT START OF TIME FRAME
SUBTRACT DEMAND FROM CAPICITY OF AQUIFER
END LOOP

FIGURE 8

ITERATIVE SCHEME-SURFACE RESERVOIR

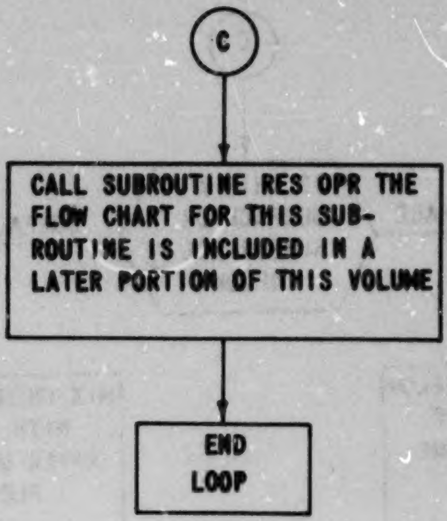

C
CALL SUBROUTINE RES OPR THE FLOW CHART FOR THIS SUBROUTINE IS INCLUDED IN A LATER PORTION OF THIS VOLUME
END LOOP

FIGURE 9

ITERATIVE SCHEME-INFLOWS

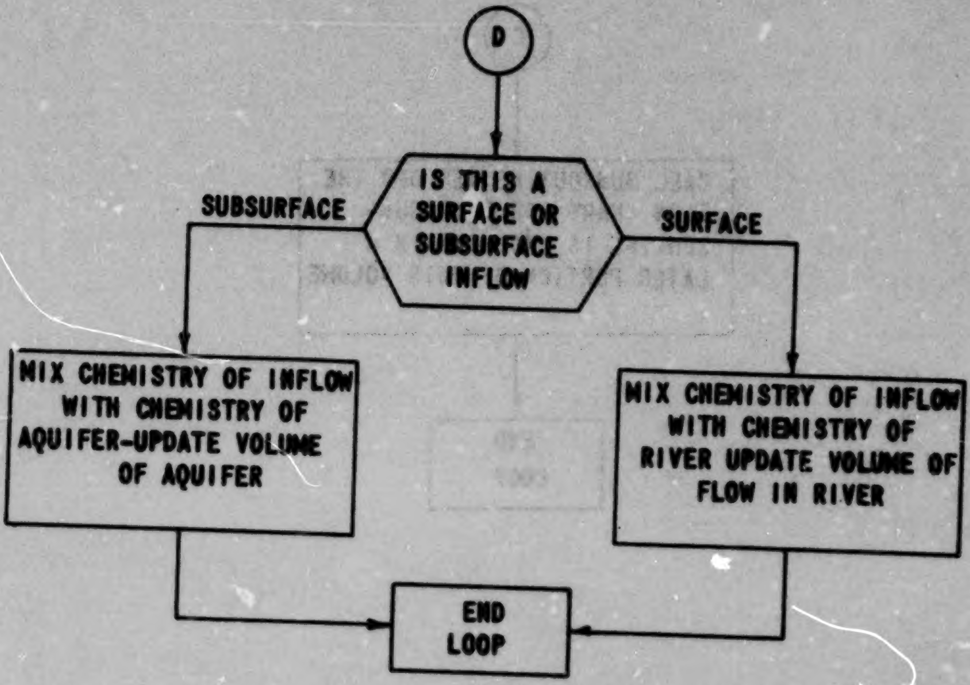

D
IS THIS A SURFACE OR SUBSURFACE INFLOW
SUBSURFACE
SURFACE
MIX CHEMISTRY OF INFLOW WITH CHEMISTRY OF AQUIFER-UPDATE VOLUME OF AQUIFER
MIX CHEMISTRY OF INFLOW WITH CHEMISTRY OF RIVER UPDATE VOLUME OF FLOW IN RIVER
END LOOP

FIGURE 10

ITERATIVE SCHEME-END OF LOOP LOGIC

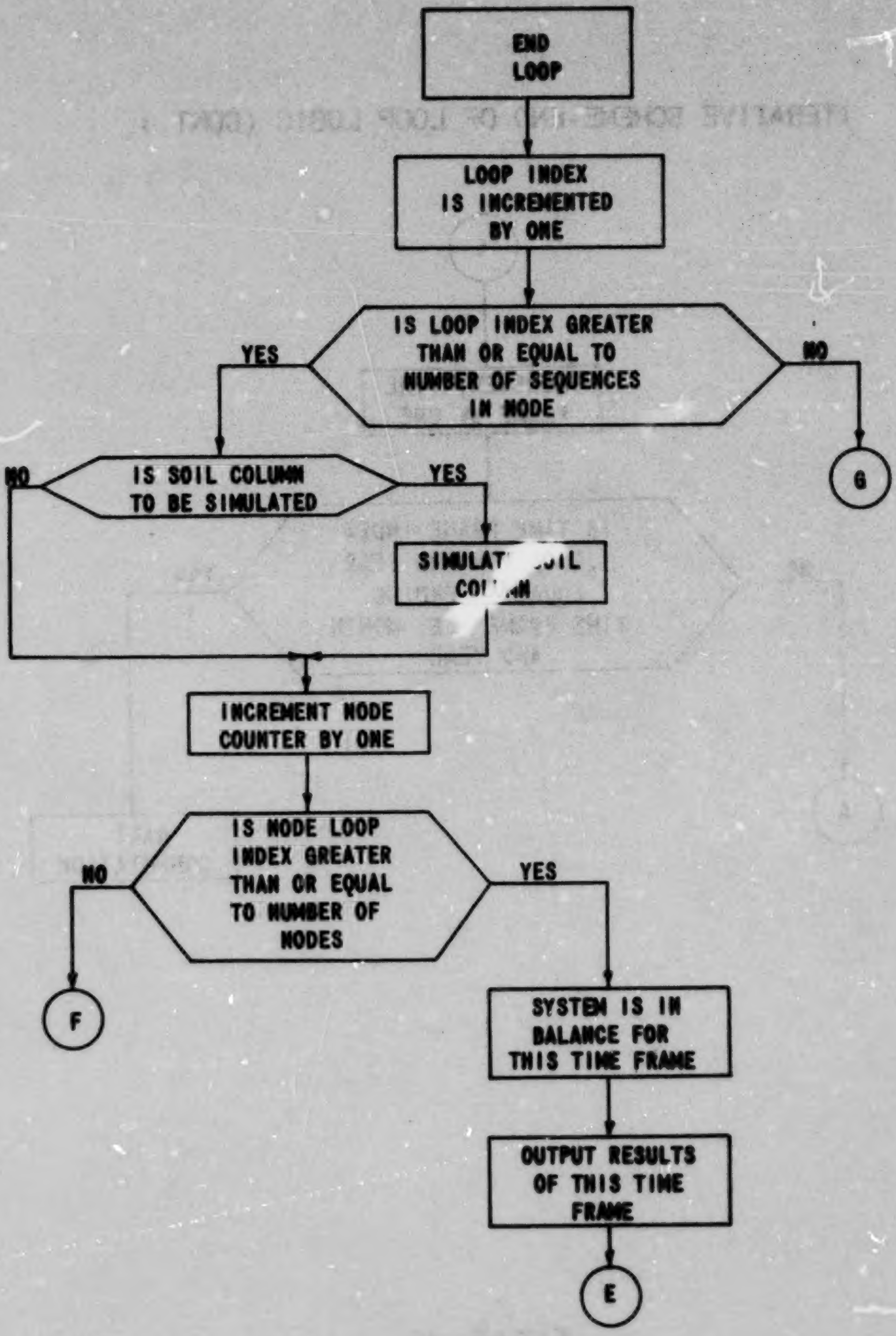

END LOOP
LOOP INDEX IS INCREMENTED BY ONE
IS LOOP INDEX GREATER THAN OR EQUAL TO NUMBER OF SEQUENCES IN NODE
YES
NO
G
IS SOIL COLUMN TO BE SIMULATED
NO
YES
SIMULATE SOIL COLUMN
INCREMENT NODE COUNTER BY ONE
IS NODE LOOP INDEX GREATER THAN OR EQUAL TO NUMBER OF NODES
NO
YES
F
SYSTEM IS IN BALANCE FOR THIS TIME FRAME
OUTPUT RESULTS OF THIS TIME FRAME
E

FIGURE 11

ITERATIVE SCHEME-END OF LOOP LOGIC (CONT.)

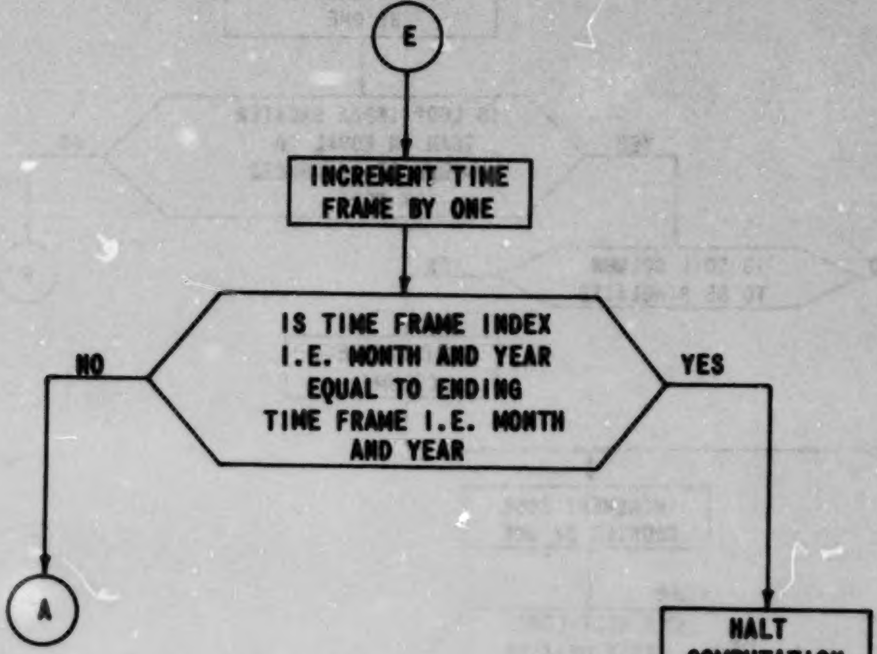

E
INCREMENT TIME FRAME BY ONE
IS TIME FRAME INDEX I.E. MONTH AND YEAR EQUAL TO ENDING TIME FRAME I.E. MONTH AND YEAR
NO
YES
A
HALT COMPUTATION

FIGURE 12

Table 1

VARIABLE NAMES OR DATA ARRAYS FOR MAIN PROGRAM

Variable name	C*	Description	Remarks or Units
BEGWR	C	Data array for beginning of time frame conditions for aquifer	See data array BEGWR
CHEMBT		Entry to subroutine CHEMGR	See subroutine CHEMGR
CHEMDM	C	Data array for chemistry of demands	See data array CHEMDM
CHEMGR		Entry to subroutine CHEMGR	See subroutine CHEMGR
CHEMRV		Entry to subroutine CHEMGR	See subroutine CHEMGR
CHEMTT		Entry to subroutine CHEMGR	See subroutine CHEMGR
COMPA		Computation aid	
COMP		Computation aid	
CONST		Computation aid	
CONVER		Entry to subroutine CONVER	See subroutine CONVER
DELTAF		Reservoir release made to meet a downstream deficit	Acre-feet
DEMAND	C	Data array for demands	See data array DEMAND
DTABLE		Entry to subroutine DTABLE	See subroutine DTABLE
GRTANK	C	Data array for volume and chemistry of aquifer	See data array GRTANK

C* = Variable names shared in common blocks

Table 1 - Continued

Variable name	C*	Description	Remarks or Units
IC		Index of number of upstream reservoirs	
IFIR		Index used to run jobs back to back redundant in this version	
INDY		Index used in calling argument for subroutine RFCOMP	See subroutine RFCOMP
IR		Read unit designation	
ISEQ		Data array for operation sequences in node	
IS		Absolute value for index of sequence operation	
IW		Write unit designation	
IYRBEG		Beginning year of study	2 digits i.e., 69,70
IYREND		Ending year of study	2 digits
IYR		Year of study during computational cycle	2 digits
JREAD		Read index for subroutine PERUSE	See subroutine PERUSE
KA		Loop index	
KFAK	C	Data array to store ranking of reservoirs	See subroutine DTABLE
KG		Computational aid	
KNODE		Node index	
KN		Loop index	

Table 1 - Continued

Variable name	C*	Description	Remarks or Units
KPRI	C	Redundant in this version	
K		Loop index	
KS		Computational aid	
KUSE		Data array for consumptive use (equivalence to CONUSE)	See data array CONUSE
KX		Computational aid	
KZ		Computational aid	
LINE		Line counter - redundant	
MINA		Beginning index for operational sequence loop in iterative scheme	
MIN		Beginning index for node sequence loop in iterative scheme	
MOBEG		Beginning month of study	2 digits i.e., JAN=01
MODE		Computational aid	
MOEND		Ending month of study	2 digits i.e., JUN=06
MO		Month or time frame of study during computation	2 digits i.e., DEC=12
NCTRL	C	Data array for the control of flow from node to node	
ND		Computational aid	
NFIND		Entry to function NFIND	See function NFIND
NPASS		Computational aid which counts passes thru each reservoir during one time frame	

Table 1 - Continued

Variable name	C*	Description	Remarks or Units
NSEG		Number of segments in any one soil column	
NSOIL		Sequence of any soil column in river basin (one per node)	
NS		Number of sequences of operation in any one node used as loop index in iterative scheme	
NUMSEQ	C	Number of sequences of operation in any one node	
OBSERV		Total of observed flows and chemistry as checks in any one node	
OBSVAL	C	Same as OBSERV	
PERUSE		Entry to read subroutine PERUSE	
PREDIC	C	Predicted flows and chemistry leaving each node	
PRELM		Computational aid to determine possible reservoir release	
QFLOW		An array used to transfer data as a part of argument	
QINFLO	C	An array used to store inflows to system	See data array QINFLO
QINRIV		An array used to store river flow and chemistry at any point in river basin	
RDATA	C	An array used to store pertinent reservoir data	See subroutine RESOPR
RESOPR		Entry to reservoir operation subroutine RESOPR	See subroutine RESOPR

Table 1 - Continued

Variable name	C*	Description	Remarks or Units
RFCOMP		Entry to return flow subroutine RFCOMP	See subroutine RFCOMP
SOILCO		Entry to monitor subroutine for soil column simulation	See subroutine SOILCO
TEMPR		An array used as a computational aid	
TEMP		A computational array	
TEST		A computational aid	
TR		Computational aid	
TTANK	C	An array used to store flows and chemistry for water to be percolated thru soil column	See data array TTANK
VERNAL		Subroutine containing the operation criteria for the VERNAL RIVER BASIN	This subroutine will be rewritten for each river basin
WRIT		Subroutine used to output results or generate report	This subroutine will be rewritten for each river basin

Table 1 - Continued

DATA ARRAYS IN MAIN PROGRAM

DATA ARRAY BEGWR (20,10)

BEGWR (J,1) = Volume of water stored in subsurface reservoir (aquifer) at beginning of time frame

BEGWR (J,2) = Concentration of calcium in aquifer in ppm

BEGWR (J,3) = Concentration of magnesium

BEGWR (J,4) = Concentration of sodium

BEGWR (J,5) = Concentration of chloride

BEGWR (J,6) = Concentration of sulfate

BEGWR (J,7) = Concentration of bicarbonate

BEGWR (J,8) = Concentration of carbonate

BEGWR (J,9) = Concentration of nitrate

BEGWR (J,10) = Concentration of total salts (TDS)

J = Node sequence

DATA ARRAY CHEMDM (20,10,10)

CHEMDM (J,K,1) = Blank

CHEMDM (J,K,2) = Concentration of calcium in water used to meet demand in ppm

CHEMDM (J,K,3) = Concentration of magnesium

CHEMDM (J,K,4) = Concentration of sodium

CHEMDM (J,K,5) = Concentration of chloride

CHEMDM (J,K,6) = Concentration of sulfate

CHEMDM (J,K,7) = Concentration of bicarbonate

Table 1 - Continued

DATA ARRAY CHEMDM (20,10,10) - Continued

CHEMDM (J,K,8) = Concentration of carbonate

CHEMDM (J,K,9) = Concentration of nitrate

CHEMDM (J,K,10) = Concentration of total salts (TDS)

J = Node sequence K = Sequence of operation in node

DATA ARRAY DEMAND 20,10,16

DEMAND (J,K,1-12) = Monthly demand in acre-feet

DEMAND (J,K,13) = Source of supply
Alpha = SUR index = 1.0 for surface supply
Alpha = GWR index = 2.0 for subsurface supply

DEMAND (J,K,14) = Use or transfer designation

Irrigation = IRR = 1.0
Municipal and Industrial = M&I = 2.0
Transfer to aquifer = GWR = 3.0
Transfer to soil column (TTANK) = GWV = 4.0
Transfer to river = SUR = 5.0
Transfer out of system = OUT = 6.0

All units are in acre-feet

DEMAND (J,K,15) = Consumptive use flag
0 = No consumptive use
1 = Consumptive use

DEMAND (J,K,16) = Actual diversion made to satisfy demand in acre-feet

J = Node sequence K = Sequence of operation in node

DATA ARRAY GRTANK (20,10)

GRTANK (J,1) = Volume of water in subsurface storage (aquifer) in acre-feet

GRTANK (J,2) = Concentration of calcium in aquifer in ppm

Table 1 - Continued

DATA ARRAY GRTANK (20,10) - Continued

GRTANK (J,3) = Concentration of magnesium

GRTANK (J,4) = Concentration of sodium

GRTANK (J,5) = Concentration of chloride

GRTANK (J,6) = Concentration of sulfate

GRTANK (J,7) = Concentration of bicarbonate

GRTANK (J,8) = Concentration of carbonate

GRTANK (J,9) = Concentration of nitrate

GRTANK (J,10) = Concentration of total salts (TDS)

J = Node index

DATA ARRAY CONUSE (20,10,30) EQUIVALANCE KUSE (20,10,30)

CONUSE (J,K,1-12) = Monthly consumptive use in acre-feet

CONUSE (J,K,13) = Conveyance and farm losses in percent of demand (see subroutine RFCOMP)

CONUSE (J,K,14) = Shortage index percent

CONUSE (J,K,15) = Shortage in acre-feet

CONUSE (J,K,19-30) = Return flow allocations and destinations

CONUSE (J,K,19,23,27)= Use or destination indicator
SUR = Return to river
GWR = Return to aquifer
GWV = Return to TTANK for percolation thru soil column

CONUSE (J,K,20,24,28)= Node number of destination

CONUSE (J,K,21,25,29)= Operation sequence of destination

Table 1 - Continued

DATA ARRAY CONUSE (20,10,30) EQUIVALANCE KUSE (20,10,30) - Continued

CONUSE (J,K,22,26,30)= Percent of total return flow allotted to each destination or use

J = Node index K = Sequence of operation in node

DATA ARRAY QINFLO (20,10,12)

QINFLO (J,K,1) = Volume of inflow in acre-feet

QINFLO (J,K,2) = Concentration of calcium in ppm

QINFLO (J,K,3) = Concentration of magnesium

QINFLO (J,K,4) = Concentration of sodium

QINFLO (J,K,5) = Concentration of chloride

QINFLO (J,K,6) = Concentration of sulfate

QINFLO (J,K,7) = Concentration of bicarbonate

QINFLO (J,K,8) = Concentration of carbonate

QINFLO (J,K,9) = Concentration of nitrate

QINFLO (J,K,10) = Concentration of total salts (TDS)

QINFLO (J,K,11) = Destination of inflow

1.0 = To river
2.0 = To aquifer
3.0 = To ponding pool above soil column (TTANK)
4.0 = To check point (observed flow and chemistry at check point to compare with predicted flow and chemistry at check point or response point).

QINFLO (J,K,12) = Units of chemical concentrations

1 = MEQ/liter
2 = Parts per million (ppm)

J = Node index K = sequence of operation in node

Table 1 - Continued

DATA ARRAY TTANK (20,10)

TTANK (J,1) = Volume of water in ponding pool above surface to percolate thru soil column in acre-feet

TTANK (J,2) = Concentration of calcium in ppm

TTANK (J,3) = Concentration of magnesium

TTANK (J,4) = Concentration of sodium

TTANK (J,5) = Concentration of chloride

TTANK (J,6) = Concentration of sulfate

TTANK (J,7) = Concentration of bicarbonate

TTANK (J,8) = Concentration of carbonate

TTANK (J,9) = Concentration of nitrate

TTANK (J,10) = Concentration of total salts (TDS)

J = Node index

DATA ARRAY BTANK (20,10)

BTANK (J,1) = Volume of water in tank immediately below soil column and above aquifer

BTANK (J,2) = Concentration of calcium in ppm

BTANK (J,3) = Concentration of magnesium

BTANK (J,4) = Concentration of sodium

BTANK (J,5) = Concentration of chloride

BTANK (J,6) = Concentration of sulfate

BTANK (J,7) = Concentration of bicarbonate

BTANK (J,8) = Concentration of carbonate

BTANK (J,9) = Concentration of nitrate

BTANK (J,10) = Concentration of total salts (TDS)

J = Node index

SUBROUTINE PERUSE

All read instructions for the model are contained within this subroutine. Also, most of the data arrays are filled or partially filled in this subroutine. The read formats were designed in a manner that will allow the input of several different types of data with the use of the same format.

A general flow chart of this subroutine is shown on Figure 13.

The index used in the PERUSE subroutine is assigned the variable name JREAD which is an integer number varying between 1 and 5. All one-time reads made for any one particular simulation are made when JREAD varies between 1 and 4.

Each of the card formats used to read the input data are shown in Table 2. Many river basin studies will not have all of the data or physical features included in the table of model input data. The lack of data or physical features for any given river basin study presents no problem as far as the read subroutine is concerned or for that matter the flow of the model.

The control cards read when JREAD=1 are probably the most difficult to explain, and yet once they are fully understood, they are simple to apply and represent the versatility of the model in general. The

FLOW CHART SUBROUTINE PERUSE

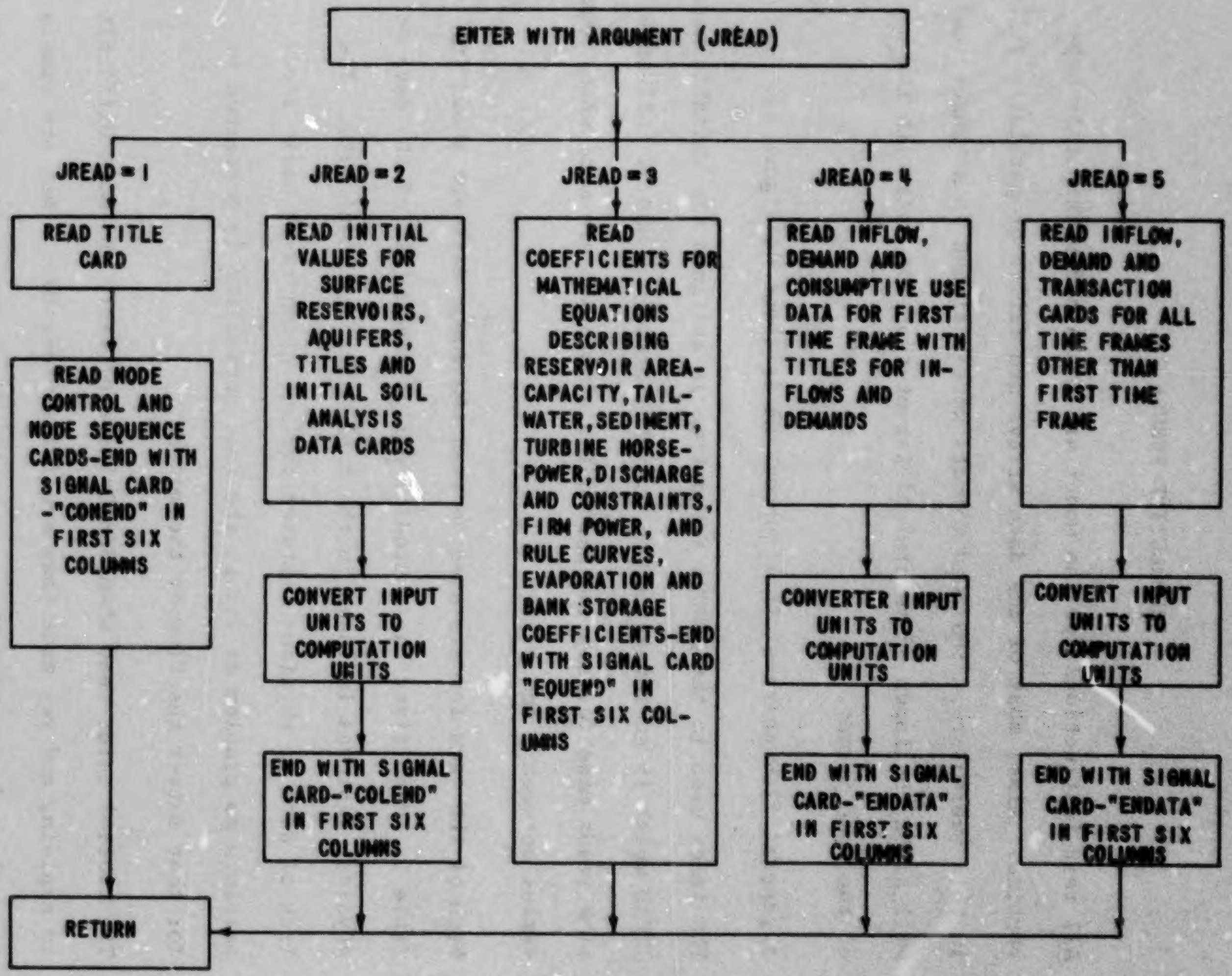

ENTER WITH ARGUMENT (JREAD)
JREAD = 1
JREAD = 2
JREAD = 3
JREAD = 4
JREAD = 5
READ TITLE CARD
READ NODE CONTROL AND NODE SEQUENCE CARDS-END WITH SIGNAL CARD -"CONEND" IN FIRST SIX COLUMNS
READ INITIAL VALUES FOR SURFACE RESERVOIRS, AQUIFERS, TITLES AND INITIAL SOIL ANALYSIS DATA CARDS
CONVERT INPUT UNITS TO COMPUTATION UNITS
END WITH SIGNAL CARD-"COLEND" IN FIRST SIX COLUMNS
READ COEFFICIENTS FOR MATHEMATICAL EQUATIONS DESCRIBING RESERVOIR AREA-CAPACITY, TAILWATER, SEDIMENT, TURBINE HORSEPOWER, DISCHARGE AND CONSTRAINTS, FIRM POWER, AND RULE CURVES, EVAPORATION AND BANK STORAGE COEFFICIENTS-END WITH SIGNAL CARD "EQUEND" IN FIRST SIX COLUMNS
READ INFLOW, DEMAND AND CONSUMPTIVE USE DATA FOR FIRST TIME FRAME WITH TITLES FOR INFLOWS AND DEMANDS
CONVERTER INPUT UNITS TO COMPUTATION UNITS
END WITH SIGNAL CARD-"ENDATA" IN FIRST SIX COLUMNS
READ INFLOW, DEMAND AND TRANSACTION CARDS FOR ALL TIME FRAMES OTHER THAN FIRST TIME FRAME
CONVERT INPUT UNITS TO COMPUTATION UNITS
END WITH SIGNAL CARD-"ENDATA" IN FIRST SIX COLUMNS
RETURN

FIGURE 13

Table 2

MODEL INPUT DATA

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
1	8A8	1-64	Title card, name of river basin study	LTITLE	None
	I16	65-80	Redundant in this version of model	KPRI	None
1	2R3	1-6	Read sentinel		CONNOD
	I3	7-9	Node number	NCTRL(J,1)	None
	I3	10-12	Node number of node immediately downstream of NCTRL(20,1)	NCTRL(J,2)	None
	I3	13-15	Sequence number in operational sequence of downstream node	NCTRL(J,3)	None
1	2R3	1-6	Read sentinel		CONSEQ
	I3	7-9	Node number		None
	I3	10-12	Number of sequential operations in node	NUMSEQ(J)	None
	20I3	13-72	Sequential operation Without sign = inflows With minus sign = demands Zero = surface reservoir	ISEQ(J,K)	None

J = Node sequence (1-20)
K = Operation sequence in node (1-20)

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
1	2R3	1-6	Read sentinel		CONWAT
	I3	7-9	Node number		
	I3	13-15	Upstream node No.	NDWTR(J,1)	
	I3	16-18	" " "	NDWTR(J,2)	
	I3	19-21	" " "	NDWTR(J,3)	
	I3	22-24	" " "	NDWTR(J,4)	
	I3	25-27	" " "	NDWTR(J,5)	
	I3	28-30	" " "	NDWTR(J,6)	
	I3	31-33	" " "	NDWTR(J,7)	
	I3	4-36	" " "	NDWTR(J,8)	
	I3	37-39	" " "	NDWTR(J,9)	
	I3	40-42	" " "	NDWTR(J,10)	
	I3	43-45	" " "	NDWTR(J,11)	
	I3	46-48	" " "	NDWTR(J,12)	
	I3	49-51	" " "	NDWTR(J,13)	
	I3	52-54	" " "	NDWTR(J,14)	
	I3	55-57	" " "	NDWTR(J,15)	
	I3	58-60	" " "	NDWTR(J,16)	
	I3	61-63	" " "	NDWTR(J,17)	
	I3	64-66	" " "	NDWTR(J,18)	
	I3	67-69	" " "	NDWTR(J,19)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	I3	70-72	Upstream node No.	NDWTR(J,20)	
J =	Node index				
1	2R3	1-6	Read sentinel		CONEND
	I3	7-9	Beginning month of study	MOBEG	2 digits
	I3	10-12	Beginning year of study	IYRBEG	2 digits
	I3	13-15	Ending month of study	MOEND	2 digits
	I3	16-18	Ending year of study	IYREND	2 digits

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
2	2R3	1-6	Read sentinel		AQUFER
	I3	10-12	Node number		
	8A8	16-79	Name of aquifer	KAQUMN(J,1-8)	

J = Node index

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
2	2R3	1-6	Read sentinel		GRTANK
	I1	9	Units indicator 1= MEQ/liter 2= PPM		
	I3	10-12	Node number		
	F6.0	16-21	Volume of aquifer in AF * 10^m	GRTANK(J,1)	
	F6.0	22-27	Calcium concentration	GRTANK(J,2)	
	F6.0	28-33	Magnesium concentration	GRTANK(J,3)	
	F6.0	34-39	Sodium concentration	GRTANK(J,4)	
	F6.0	40-45	Chloride concentration	GRTANK(J,5)	
	F6.0	46-51	Sulfate concentration	GRTANK(J,6)	
	F6.0	52-57	Bicarbonate concentration	GRTANK(J,7)	
	F6.0	58-63	Carbonate concentration	GRTANK(J,8)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F6.0	64-69	Nitrate concentration	GRTANK(J,9)	
	F6.0	70-75	Total salts (TDS)	GRTANK(J,10)	
	I2	76-77	Month		
	I1	78	"m" a power of 10		
	I2	79-80	Year		
J =	Node index				
2	2R3	1-6	Read sentinel		SURRES
	I3	10-12	Node number		
	8A8	16-79	Name of reservoir	KSURNM(J,1-8)	
J =	Node index				
2	2R3	1-6	Read sentinel		RESDAT
	I2	7-8	Operation sequence number in node	RDATA(J,2)	
	I3	10-12	Node number	RDATA(J,1)	
	F6.0	16-21	Volume of reservoir in AF * 10^m		
	F6.0	22-27	Maximum reservoir capacity AF * 10^m	RDATA(J,11)	
	F6.0	28-33	Minimum reservoir release cfs * 10^m	RDATA(J,12)	
	F6.0	34-39	Maximum release w/o spill cfs * 10^m	RDATA(J,13)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F6.0	40-45	Maximum release w/o spill cfs * 10^m	RDATA(J,14)	
	F6.0	46-51	Sediment deposited in reservoir AF * 10^m	RDATA(J,20)	
	I1	78	"m" a power of 10		
J =	Node index				
2	2R3	1-6	Read sentinel		RESCHM
	I1	9	Units indicator 1 = MEQ/Liter 2 = PPM		
	I3	10-12	Node number		
	F6.0	22-27	Calcium concentration	RDATA(J,101)	
	F6.0	28-33	Magnesium concentration	RDATA(J,102)	
	F6.0	34-39	Sodium concentration	RDATA(J,103)	
	F6.0	40-45	Chloride concentration	RDATA(J,104)	
	F6.0	46-51	Sulfate concentration	RDATA(J,105)	
	F6.0	52-57	Bicarbonate concentration	RDATA(J,106)	
	F6.0	58-63	Carbonate concentration	RDATA(J,107)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F6.0	64-69	Nitrate concentration	RDATA(J,108)	
	F6.0	70-75	Total salts (TDS)	RDATA(J,109)	

J = Node index

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
2	2R3	1-6	Read sentinel		COLBEG
	I2	7-8	Number of segments in soil column	NSEG(J)	
	I3	10-12	Node number		

J = Node index

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
2	2R3	1-6	Read sentinel		COLSEG
	I3	7-9	Node number		
	I3	10-12	Segment number		
	F5.0	13-17	Calcium concentration in MEQ/liter	SOIL(J,K,1)	
	F5.0	18-22	Magnesium concentration in MEQ/liter	SOIL(J,K,2)	
	F5.0	23-27	Sodium concentration in MEQ/liter	SOIL(J,K,3)	
	F5.0	28-32	Chloride concentration in MEQ/liter	SOIL(J,K,4)	
	F5.0	33-37	Sulfate concentration in MEQ/liter	SOIL(J,K,5)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F5.0	38-42	Bicarbonate concentration in MEQ/liter	SOIL(J,K,6)	
	F5.0	43-47	Carbonate concentration in MEQ/liter	SOIL(J,K,7)	
	F5.0	48-52	Nitrate concentration in MEQ/liter	SOIL(J,K,8)	
	F3.0	53-55	Soil/water ratio of extract	SOIL(J,K,9)	
	F5.0	56-60	Volume of water in segment in milliliters	SOIL(J,K,10)	
	F5.0	61-65	Cation exchange capacity in MEQ/100 gr	SOIL(J,K,11)	
	F5.0	66-70	Concentration of Gypsum Dihydrate in units of MEQ/100 gr	SOIL(J,K,12)	
	F1.0	71	Lime indicator 0 = No lime present 1 = Lime present	SOIL(J,K,13)	
	F4.0	72-75	Bulk density of soil in segment in units of grams/cubic centimeter	SOIL(J,K,14)	
	F5.0	76-80	Length of soil segment in centimeters	SOIL(J,K,15)	

J = Node index

K = Operation sequence in node

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
2	2R3	1-6	Read sentinel for end JREAD=2		COLEND
3	2R3	1-6	Read sentinel		EQURES
	I4	7-10	Node number		
	I3	11-13	Index "L" in array sequence		
	F12.0	14-25	Base elevation in feet above msl	RDATA(J,K,L)	
	I3	26-28	Index "L" in array sequence		
	F12.0	29-40	Coefficient A_o in polynomial	RDATA(J,K,L)	
	I3	41-43	Index "L" in array sequence		
	F12.0	44-55	Coefficient A_1 in polynomial	RDATA(J,K,L)	
	I3	56-58	Index "L" in array sequence		
	F12.0	59-70	Coefficient A_2 in polynomial	RDATA(J,K,L)	

Polynomial - Capacity = $A_0 + A_1H + A_2H^2$ - where H = height above base elevation

J = Node index

K = Operation sequence in node

3	2R3	1-6	Read sentinel		EQUSED
	I4	7-10	Node number		

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	I3	11-13	Index = 15		
	F12.0	14-25	Coefficient "A" in first equation	RDATA(J,K,15)	
	I3	26-28	Index = 16		
	F12.0	29-40	Coefficient "B" in first equation	RDATA(J,K,16)	
	I3	41-43	Index = 17		
	F12.0	44-55	Coefficient "A" in second equation	RDATA(J,K,17)	
	I3	56-58	Index = 18		
	F12.0	59-70	Coefficient "B" in second equation	RDATA(J,K,18)	
	F10.0	71-80	Spline point for equations in cfs	RDATA(J,K,19)	

Equation - Sediment = AQ^B

J = Node index K = Operation sequence in node

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
3	2R3	1-6	Read sentinel		EQUTWR
	I4	7-10	Node number		
	I3	11-13	Index = 1		
	F12.0	14-25	Base elevation for tailwater curve in feet above msl	TDATA(J,1)	
	I3	26-28	Index = 2		
	F12.0	29-40	Coefficient A_0 in polynomial	TDATA(J,2)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	I3	41-43	Index = 3		
	F12.0	44-55	Coefficient A_1 in polynomial	TDATA(J,3)	
	I3	56-58	Index = 4		
	F12.0	59-70	Coefficient A_2 in polynomial	TDATA(J,4)	

Polynomial - Tailwater elevation = Base elevation + $(A_0+A_1H+A_2H^2)$
where H = height above base elevation

J = Node index

3	2R3	1-6	Read sentinel		EQUEFF
	I4	7-10	Node number		
	I3	11-13	Index = 1		
	F12.0	14-25	Coefficient A_o in polynomial	ENERGY(J,1)	
	I3	26-28	Index = 2		
	F12.0	29-40	Coefficient A_1 in polynomial	ENERGY(J,2)	
	I3	41-43	Index = 3		
	F12.0	44-55	Coefficient A_2 in polynomial	ENERGY(J,3)	

Polynomial - Horsepower = $A_0+A_1H+A_2H^2$ where H = Net head

J = Node index

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
3	2R3	1-6	Read sentinel		EQUEFF
	I4	7-10	Node number		
	I3	11-13	Index = 5		
	F12.0	14-25	Coefficient A_0 in polynomial	ENERGY(J,5)	
	I3	26-28	Index = 6		
	F12.0	29-40	Coefficient A_1 in polynomial	ENERGY(J,6)	
	I3	41-43	Index = 7		
	F12.0		Coefficient A_2 in polynomial	ENERGY(J,7)	

Polynomial - Discharge (cfs) at full gate = $A_0+A_1H+A_2H^2$
where H = Net Head. J = Node index

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
3	2R3	1-6	Read sentinel		EQUCAP
	I4	7-10	Node number		
	I3	11-13	Index = 1		
	F12.0	14-25	Number of generator units in powerplant	CAPBAB(J,1)	
	I3	26-28	Index = 2		
	F12.0	29-40	Generator rating (KV-A)	CAPBAB(J,2)	
	I3	41-43	Index = 3		

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F12.0	44-55	Power factor (dimensionless)	CAPBAB(J,3)	
	I3	56-58	Index = 4		
	F12.0	59-70	Percent of overload	CAPBAB(J,4)	
J = Node index					
3	2R3	1-6	Read sentinel		EQUCAP
	I4	7-10	Node number		
	I3	11-13	Index = 6		
	F12.0	14-25	Generator efficiency in %	CAPBAB(J,6)	
	I3	26-28	Index = 7		
	F12.0	29-40	Maximum head in ft	CAPBAB(J,7)	
	I3	41-43	Index = 8		
	F12.0	44-55	Minimum head in ft	CAPBAB(J,8)	
J = Node index					

Three cards with identical format are used for the firm power requirements on a monthly time frame for a one-year period.

3	2R3	1-6	Read sentinel		EQUPOW
	I4	7-10	Node number		
	I3	11-13	Index = 1, 5, 9	PDATA(J,Index)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F12.0	14-25	Firm power requirement in KWH for months JAN, MAY, SEPT		
	I3	26-28	Index = 2, 6, 10		
	F12.0	29-40	Firm power requirement in KWH for months FEB, JUNE, OCT	PDATA(J,Index)	
	I3	41-43	Index = 3, 7, 11		
	F12.0	44-55	Firm power requirement in KWH for months MARCH, JULY, NOV	PDATA(J,Index)	
	I3	56-58	Index = 4, 8, 12		
	F12.0	59-70	Firm power requirement in KWH for months APRIL, AUG, DEC		

J = Node index

Three cards with identical format are used for the reservoir rule curves. These curves can either be in terms of reservoir capacity in acre-feet or reservoir water surface elevation in feet above mean sea level on a monthly time frame for a one-year period.

3	2R3	1-6	Read sentinel		EQURUL
	I4	7-10	Node number		
	I3	11-13	Index = 1, 5, 9	RULE(J,Index)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F12.0	14-25	Reservoir rule curve for months JAN, MAY, SEPT		
	I3	26-28	Index = 2, 6, 10		
	F12.0	29-40	Reservoir rule curve for months FEB, JUNE, OCT	RULE(J,Index)	
	I3	41-43	Index = 3, 7, 11		
	F12.0	44-55	Reservoir rule curve for months MAR, JULY, NOV	RULE(J,Index)	
	I3	56-58	Index = 4, 8, 12		
	F12.0	59-70	Reservoir rule curve for months APRIL, AUG, DEC		
	*F10.0	71-80	Indicator 0 = Capacities 1 = Elevations	RULE(J,13)	

*On last card only.

J = Node index

Three cards with identical format are used for the reservoir surface evaporation losses in feet per acre of area on a monthly time frame for a one-year period.

3	2R3	1-6	Read sentinel		EQUEVP
	I4	7-10	Node number		
	I3	11-13	Index = 1, 5, 9		

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F12.0	14-25	Reservoir evaporation in feet per acre area for months JAN, MAY, SEPT	CONEVP(J,Index)	
	I3	26-28	Index = 2, 6, 10		
	F12.0	29-40	Reservoir evaporation in feet per acre area for months FEB, JUNE, OCT	CONEVP(J,Index)	
	I3	41-43	Index = 3, 7, 11		
	F12.0	44-55	Reservoir evaporation in feet per acre area for months MAR, JULY, NOV	CONEVP(J,Index)	
	I3	56-58	Index = 4, 8, 12		
	F12.0	59-70	Reservoir evaporation in feet per acre area for months APRIL, AUG, DEC	CONEVP(J,Index)	

J = Node index

Three cards with identical format are used for the reservoir changes in bank storage in decimal units of change in capacity per monthly time frame for a one-year period.

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
3	2R3	1-6	Read sentinel		EQUBNK
	I4	7-10	Node number		

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS		VARIABLE NAME OR ARRAY	IDENTIFIER
	I3	11-13	Index = J		
	F12.0	14-25	Reservoir bank storage as a decimal	BANKCO(J)	
	I3	26-28	Index = J		
	F12.0	29-40	Reservoir bank storage as a decimal	BANKCO(J)	
	I3	41-43	Index = J		
	F12.0	44-55	Reservoir bank storage as a decimal	BANKCO(J)	
	I3	56-58	Index = J		
	F12.0	59-70	Reservoir bank storage as a decimal	BANKCO(J)	

J = Node index

JREAD	FORMAT	CARD COLUMNS		VARIABLE NAME OR ARRAY	IDENTIFIER
3	2R3	1-6	Read sentinel for end of JREAD = 3		EQUEND
* 4	2R3	1-6	Read sentinel		SURQIN
	I2	7-8	Operation sequence number in node		
	I3	10-12	Node number		

*This card is read for first time frame only. QINFLO card must follow this card.

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	8A8	16-79	Alphanumeric title of inflow	KQINNM(J,K,L)	
J = Node index		K = Operation sequence in node		L = 1-8	
4 or 5	2R3	1-6	Read sentinel		QINFLO
	I2	7-8	Operation sequence number in node		
	I1	9	Chemistry units indicator 1 = MEQ/Liter 2 = PPM	QINFLO(J,K,12)	
	I3	10-12	Node number		
	R3	13-15	Alpha destination indicator SUR = Surface source = 1.0 GWR = Subsurface source = 2.0 GWV = Redundant in this version CHK = Inflow check point = 4.0	QINFLO(J,K,11)	
	F6.0	16-21	Volume of inflow in AF * 10^m	QINFLO(J,K,1)	
	F6.0	22-27	Calcium concentration	QINFLO(J,K,2)	
	F6.0	28-33	Magnesium concentration	QINFLO(J,K,3)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	F6.0	34-39	Sodium concentration	QINFLO(J,K,4)	
	F6.0	40-45	Chloride concentration	QINFLO(J,K,5)	
	F6.0	46-51	Sulfate concentration	QINFLO(J,K,6)	
	F6.0	52-57	Bicarbonate concentration	QINFLO(J,K,7)	
	F6.0	58-63	Carbonate concentration	QINFLO(J,K,8)	
	F6.0	64-69	Nitrate concentration	QINFLO(J,K,9)	
	F6.0	70-75	Total salts in ppm (TDS)	QINFLO(J,K,10)	
	I2	76-77	Month		2 digits
	I1	78	"m" a power of 10		
	I2	79-80	Year		2 digits

J = Node index K = Operation sequence in node

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
* 4	2R3	1-6	Read sentinel		SURDEM
	I2	7-8	Operation sequence number in node		
	I3	10-12	Node number		
	8A8	16-79	Alphanumeric title of demand	KDEMNM(J,K,L)	

J = Node index K = Operation sequence in node L = 1-8

*This card is read for first time only. Demand card (i.e., DEMSUR or DEMGWR) must follow this card.

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
4 or 5	R3	1-3	Read sentinel		DEM
	R3	4-6	Read sentinel for source of demand	DEMAND (J,K,13)	SUR = Surface demand = 1.0 GWR = Subsurface demand = 2.0
	I2	7-8	Operation sequence number in node		
	I1	9	Input indicator where 1 indicates consumptive card to follow and 0 indicates no consumptive use card to follow		
	I3	10-12	Node number		
	R3	13-15	Alpha indicator for destination of demand IRR = Irrigation = 1.0 MAI = Municipal or industrial = 2.0 GWR = Aquifer = 3.0 GWV = Ponding pool above soil column (TTANK) = 4.0 SUR = River = 5.0 OUT = Demand leaves river basin = 6.0	DEMAND (J,K,14)	
	F6.0	16-21	Volume of demand in AF * 10^m	DEMAND (J,K,L)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	I2	76-77	Month		2 digits
	I1	78	"m" a power of 10		

J = Node index K = Operation sequence in node L = month(1-12)

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
4 or 5	R6	1-6	Read sentinel		CONUSE
	I3	7-9	Node number		
	I2	10-11	Operation sequence number in node		
	F9.0	12-20	Volume of consumptive use in acre-feet	CONUSE (J,K,L)	
	F3.0	21-23	Conveyance and farm losses in %	CONUSE (J,K,13)	
	F3.0	24-26	Shortage index in percent	CONUSE (J,K,14)	
Block #1	R3	27-29	Destination of return flow. Block #1 - SUR = Return to river GWR = Return to aquifer GWV = Return to ponding pool above soil column (TTANK)	KUSE (J,K,19)	
	I3	30-32	Node number of destination of return	KUSE (J,K,20)	

Table 2 - Continued

JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
Block #1	I2	33-34	Operation sequence number in node of return	KUSE (J,K,21)	
	I3	35-37	Percent of return allocated to this destination	KUSE (J,K,22)	
Block #2	R3	38-40	Second destination of return flow (see Block #1)	KUSE (J,K,23)	
	I3	41-43	Node number of destination of return	KUSE (J,K,24)	
	I2	44-45	Operation sequence number in node of return	KUSE (J,K,25)	
	I3	46-48	Percent of return allocated to this destination	KUSE (J,K,26)	
Block #3	R3	49-51	Third destination return flow (See Block #1)	KUSE (J,K,27)	
	I3	52-54	Node number of destination of return	KUSE (J,K,28)	
	I2	55-56	Operation sequence number in node of return	KUSE (J,K,29)	
	I3	57-59	Percent of return allocated to this destination	KUSE (J,K,30)	

Table 2 - Continued

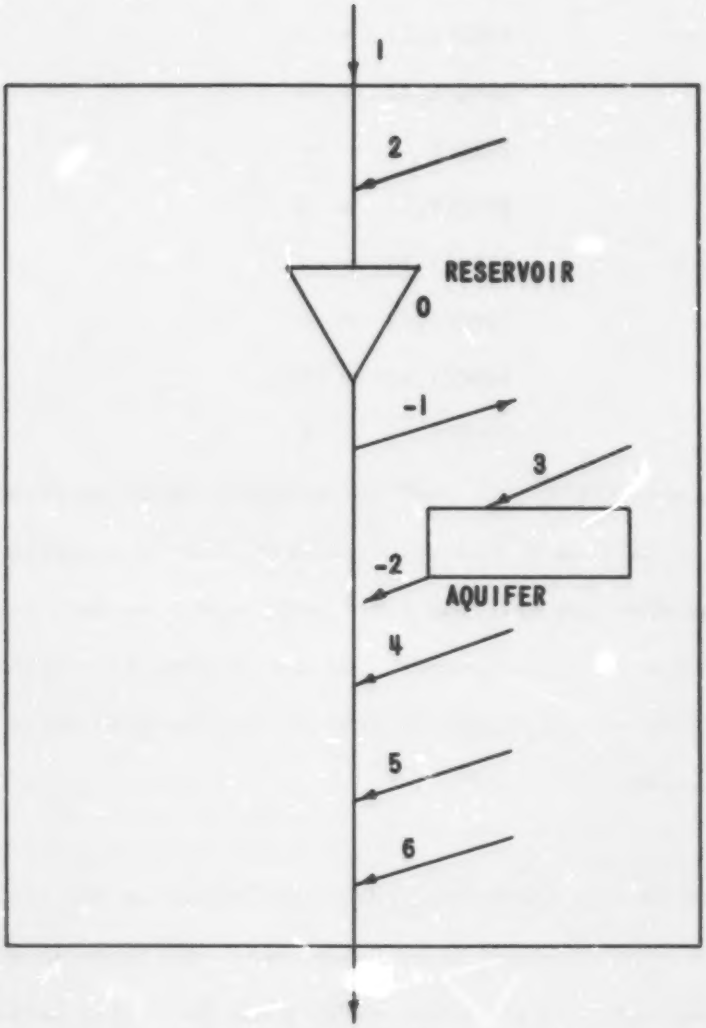
JREAD	FORMAT	CARD COLUMNS	DESCRIPTION	VARIABLE NAME OR ARRAY	IDENTIFIER
	I2	76-77	Month		2 digits
	I2	79-80	Year		2 digits
J = Node sequence			K = Operation sequence in node		
4	2R3	1-6	Read sentinel		ENDATA
5	2R3	1-6	Read sentinel		TRNACT
	I3	10-12	Node number		
	F6.0	16-21	Index in array		
	F6.0	22-27	Variable or parameter		
5	2R3	1-6	Read sentinel		ENDATA

discussion of the main program includes pictorial representations of a three node river basin and a pictorial representation of an operation sequence in a node. The flow from node to node is represented with the use of the CONNOD cards; the data contained on these cards are stored in the array NCTRL(20,3). An example of the use of the NCTRL array is as follows for the six node river basin shown on Figure 14.

Node number	Downstream node number	Operation sequence number
NCTRL(1,1)=101	NCTRL(1,2)=104	NCTRL(1,3)=3
NCTRL(2,1)=102	NCTRL(2,2)=103	NCTRL(2,3)=1
NCTRL(3,1)=103	NCTRL(3,2)=104	NCTRL(3,3)=1
NCTRL(4,1)=104	NCTRL(4,2)=106	NCTRL(4,3)=1
NCTRL(5,1)=105	NCTRL(5,2)=106	NCTRL(5,3)=5
NCTRL(6,1)=106	NCTRL(6,2)= 0	NCTRL(6,3)=1

The next set of control cards CONSEQ, as shown in Table 2, controls the sequence of operations in any particular node, and the data contained on these cards are stored in the arrays NUMSEQ(20) and ISEQ(20,20). An example node is shown on Figure 14, and the arrays NUMSEQ and ISEQ would be filled as follows:

EXAMPLE OPERATION SEQUENCE-NODE 2


1
2
RESERVOIR
0
-1
3
-2
AQUIFER
4
5
6

1-	Surface inflow from Node 1
2-	Tributary inflow
-1-	Irrigation demand
3-	Return flow to aquifer
-2-	Transfer of flow aquifer to river
4-	Inflow to river from aquifer
5-	Tributary inflow
6-	Tributary inflow

FIGURE 14

NUMSEQ(1) = 9

ISEQ(1,1) = 1

ISEQ(1,2) = 2

ISEQ(1,3) = 0

ISEQ(1,4) = -1

ISEQ(1,5) = 3

ISEQ(1,6) = -2

ISEQ(1,7) = 4

ISEQ(1,8) = 5

ISEQ(1,9) = 6

The control cards CONWAT are used to designate which upstream nodes can be used to satisfy a deficit of surface flow in a particular node. It is obvious that the upstream nodes must have a surface reservoir to supply such a deficit; however, for the purpose of completing these data cards it is not important to know if the upstream nodes have the reservoir feature.

The data contained on the CONWAT cards are stored in the array NDWTR(20,20). The six-node river basin shown on Figure 15 will again be used to indicate how the array NDWTR would be filled beginning with Node #101 as node sequence 1. This array would appear as follows:

EXAMPLE
RIVER BASIN WITH SIX NODES

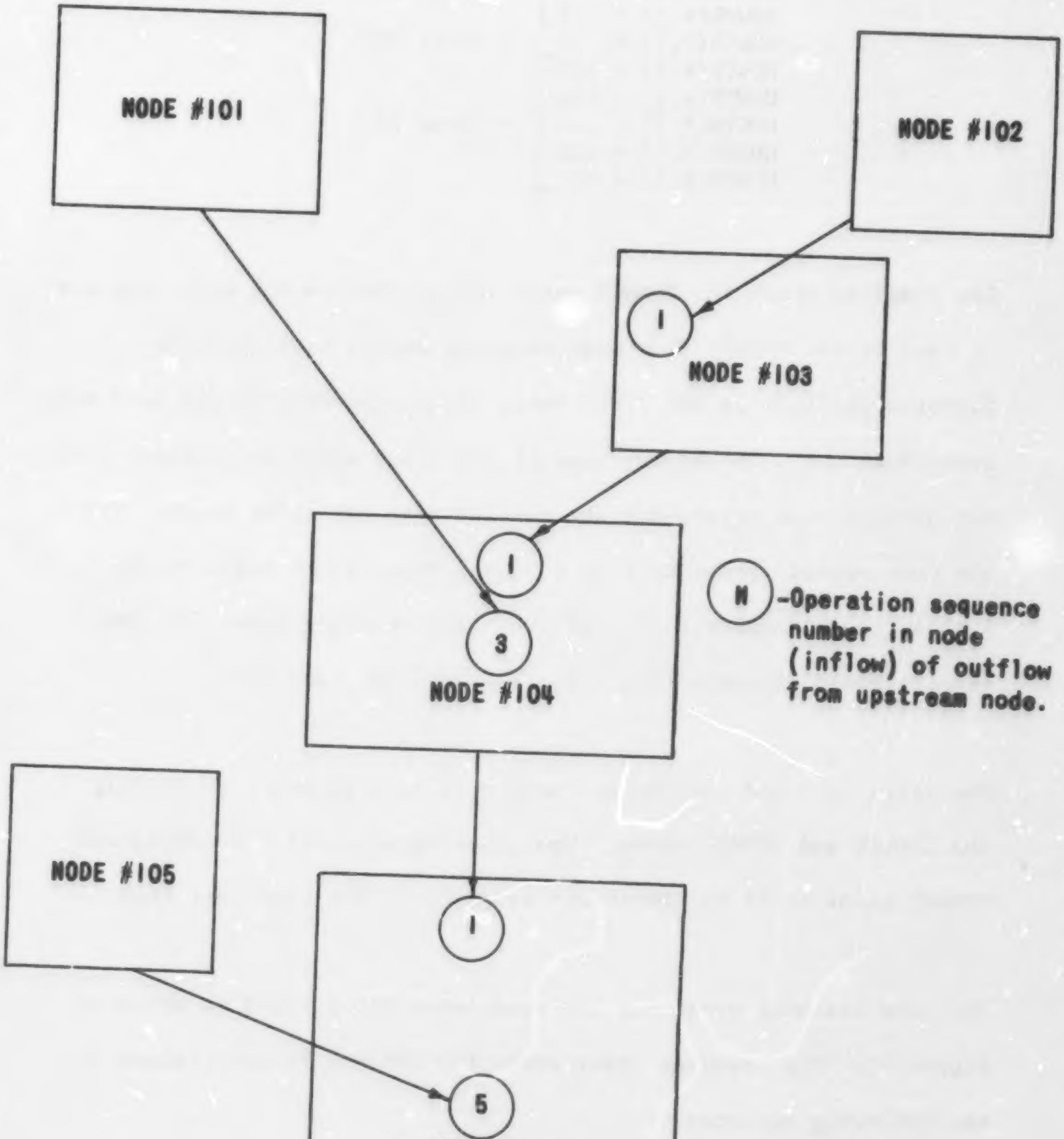

NODE #101
NODE #102
1
NODE #103
1
3
NODE #104
N
-Operation sequence number in node (inflow) of outflow from upstream node.
NODE #105
1
5
NODE #106

FIGURE 15

NDWTR(1,1) = 0 (Node 101)
NDWTR(2,1) = 0 (Node 102)
NDWTR(3,1) = 102 (Node 103)
NDWTR(4,1) = 103
NDWTR(4,2) = 102 -- (Node 104)
NDWTR(4,3) = 101
NDWTR(5,1) = 0 (Node 105)
NDWTR(6,1) = 105
NDWTR(6,2) = 104
NDWTR(6,3) = 103 -- (Node 106)
NDWTR(6,4) = 102
NDWTR(6,5) = 101

The order in which the CONNOD cards are stacked is the node sequence as used by the model. The node sequence begins with the node farthest upstream in the river basin and continues with the next node downstream until the ending node of the river basin is reached. The end of this node represents the outflow from the river basin. The six node example shown on Figure 15 has four branch nodes to the mainflow nodes numbered 104 and 106. The stacking order for this example would be nodes 101, 102, 103, 104, 105, and 106.

The title card and the CONNOD cards must be read prior to reading the CONSEQ and CONWAT cards. The stacking order of the CONSEQ and CONWAT cards is of no importance once the CONNOD cards are read.

The card stacking order for the read index JREAD = 1-3 is shown on Figure 16. The stacking order shown for JREAD=2 is constrained by the following sequences.

STACKING OF DATA DECK FOR JREAD = 1-3

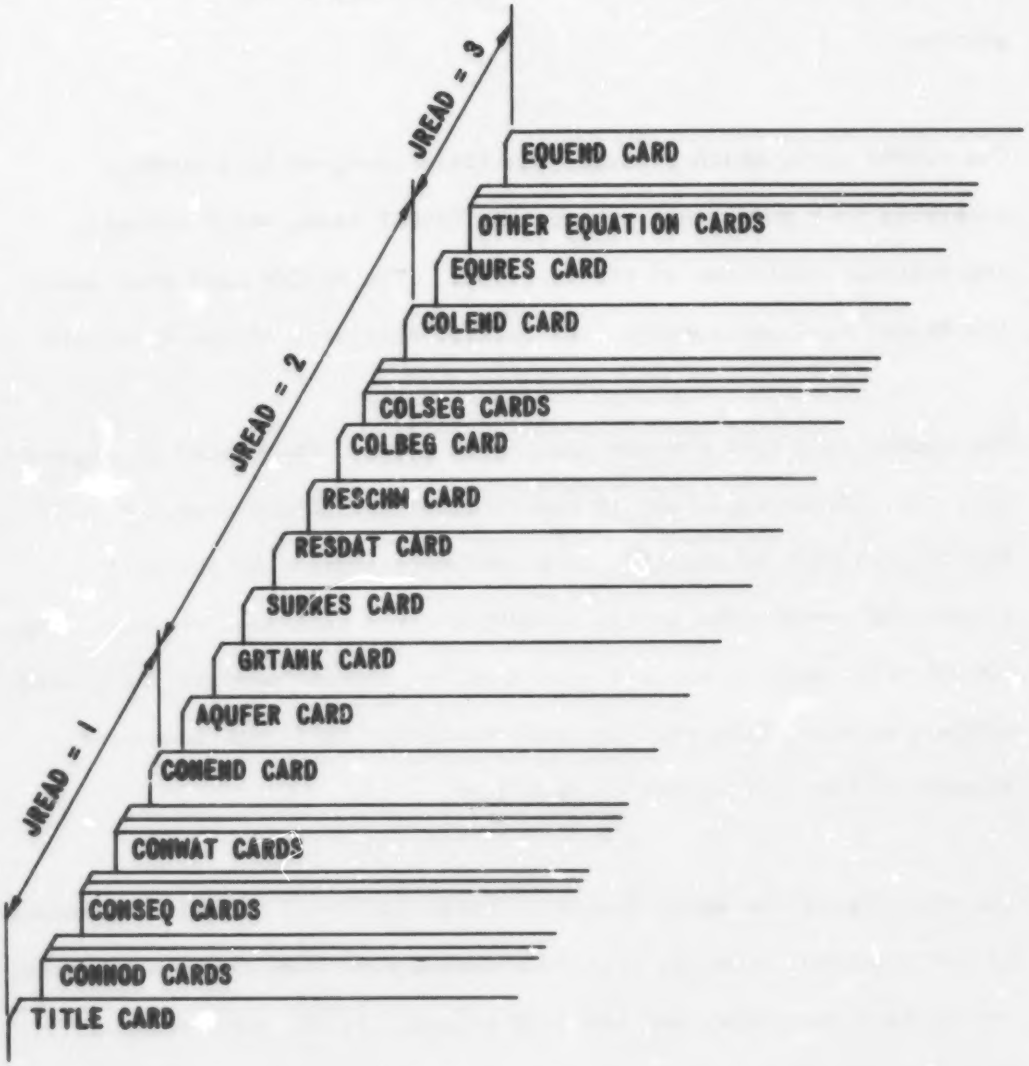

JREAD = 3
EQUEND CARD
OTHER EQUATION CARDS
EQURES CARD
COLEND CARD
JREAD = 2
COLSEG CARDS
COLBEG CARD
RESCHM CARD
RESDAT CARD
SURRES CARD
GRTANK CARD
AQUFER CARD
JREAD = 1
CONEND CARD
CONWAT CARDS
CONSEQ CARDS
CONNOD CARDS
TITLE CARD

FIGURE 16

The AQUFER card, which contains the title assigned to the aquifer (subsurface reservoir) in a node, must precede the GRTANK card, which contains the initial volume and chemistry of the particular aquifer.

The SURRES card, which contains the title assigned to a surface reservoir in a node, must precede the RESDAT card, which contains the initial conditions of the reservoir. The RESCHM card must follow the RESDAT card and contains the initial chemistry of the reservoir.

The COLBEG card must precede the COLSEG cards. The number of segments in a soil column in a node is contained on the COLBEG card. A COLSEG card must be read for each and every segment of the soil column and contain the initial conditions for each soil segment. The COLSEG cards must be stacked such that the segment nearest the ground surface is read first and the order continued until the lowermost segment in the soil column is read last.

The stacking of the above described cards according to node sequence is not required; however, each node cannot have more than one aquifer, one surface reservoir, and one soil column. In the same note, a node may contain as little as none or as many as all three of the above described features.

The equation cards read when the read index JREAD=3 are the coefficients to mathematical equations used to represent the relationship of any two variables. Mathematical equations are used to represent the capacity and area of a reservoir as a function of reservoir water surface elevation, tailwater as a function of reservoir discharge, etc. These mathematical formulations will be discussed in greater detail in later portions of this volume as they pertain to specific subroutines or functions. Here again the stacking of the equation cards with reference to node sequence is not required.

The next group of cards in the stacking order are those read when the read index JREAD=4. The stacking diagram for this read index is shown on Figure 17 . Many of types of data read when read index JREAD=4 will also be read when the read index JREAD=5.

When JREAD=4 the names or titles of all inflows and demands in the river basin must precede the actual inflow or demand data cards. This requirement pertains only to the data for the first time frame.

The SURQIN card contains the title or name of the inflow source. The data, including volume and chemistry of inflow source, are contained on the QINFLO card.

The SURDEM card contains the title or name of the demand requirement from a surface or subsurface source. The DEMSUR card contains the

STACKING OF DATA DECK FOR JREAD = 4-5

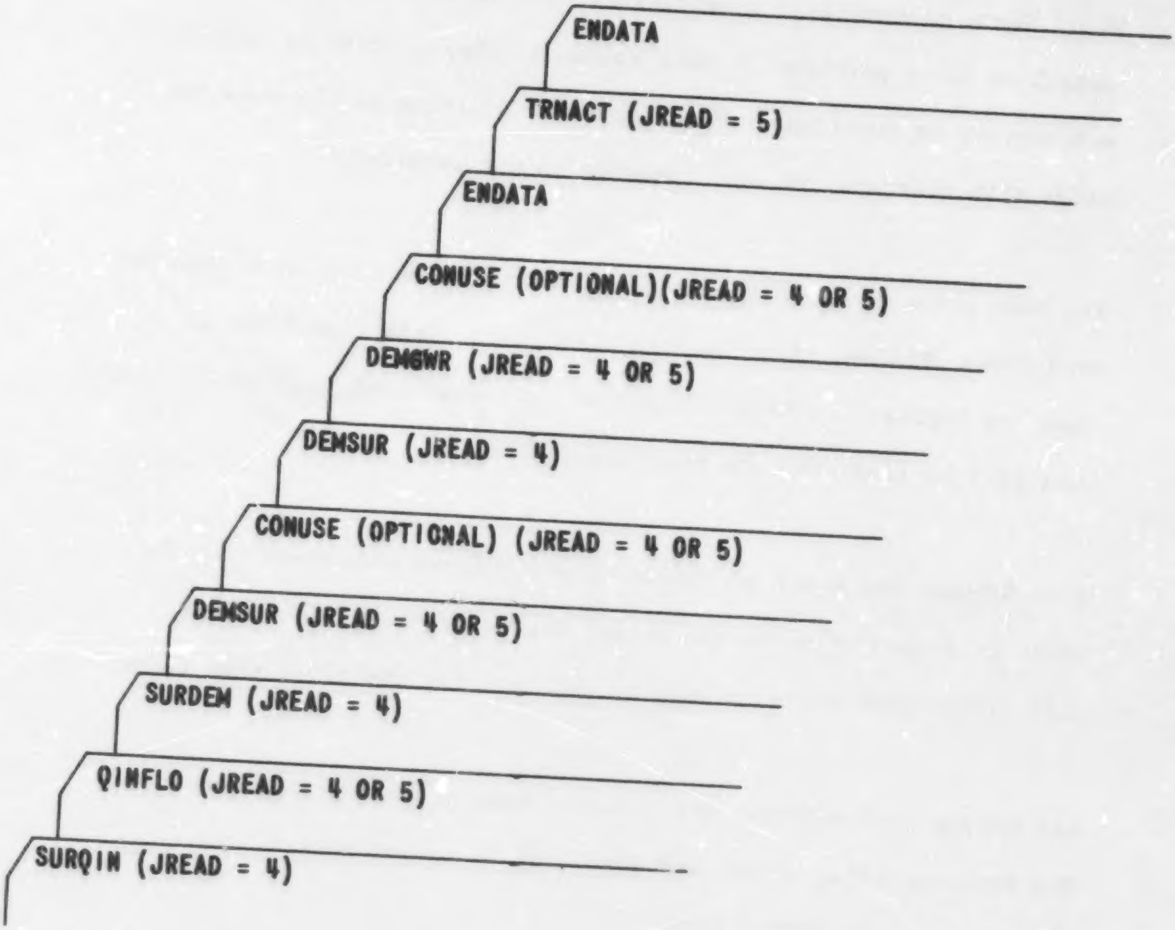

ENDATA
TRNACT (JREAD = 5)
ENDATA
CONUSE (OPTIONAL)(JREAD = 4 OR 5)
DEMGWR (JREAD = 4 OR 5)
DEMSUR (JREAD = 4)
CONUSE (OPTIONAL) (JREAD = 4 OR 5)
DEMSUR (JREAD = 4 OR 5)
SURDEM (JREAD = 4)
QINFLO (JREAD = 4 OR 5)
SURQIN (JREAD = 4)

FIGURE 17

volume of demand from a surface source and an indicator if a consumptive use or transfer card is to follow; i.e., a CONUSE card. The DEMGWR card has the same information as that of the DEMSUR card except it relates to a demand from a subsurface source. When the QINFLO, DEMSUR, DEMGWR, and CONUSE cards are read for any other time frame, except the first time frame, they are read when the read index JREAD=5 and are not preceded by the name cards SURQIN and SURDEM. The maintenance of node sequence in stacking these cards is not required.

All cards read during the first time frame are read when the read index JREAD = 1-4. The transaction cards TRNACT can be read during any time frame other than the first time frame when read index JREAD=5. The transaction cards are used to change one variable or parameter per card for such physical features as surface reservoirs and powerplants.

The variables used in this subroutine are either self-explanatory or are defined in other portions of this volume.

The various arrays used to store titles or names of surface or subsurface facilities, sources of inflow, and demand requirements are simply eight words of alphanumeric information representing these various titles or names; i.e., KSURNM(20,8) = Titles of surface reservoirs and KAQUNM(20,8) = Titles of subsurface reservoirs of one per each node for 20 nodes. The arrays used to store the eight-word titles of inflow sources and demand requirements are three dimensional to accommodate ten inflows and ten demands per node; i.e., KQINNM(20,10,8) is used to store inflow titles and KDEMNM(20,10,8) is used to store demand titles.

SUBROUTINE WRIT

This subroutine was written for the report requirements for the Vernal Project, Utah validation study.

A subroutine such as this will have to be written for each specific river basin studied and in many cases several different reports will be required for the same river basin. In this respect, some applications have been made where pertinent arrays were dumped on tape or other peripheral equipment at the end of each time frame, and an editing routine was developed for the desired report generation.

The description of the report generating routine for the Vernal Project Study would not be of a benefit for the general use of the model and, therefore, will not be included in this volume. However, a listing of the WRIT subroutine for the Vernal Project is included in the program listing for the model which is shown in a subsequent portion of this volume.

SUBROUTINE RESOPR

This subroutine is used to simulate the operation of a surface reservoir in a node. No more than one reservoir can be included in any one node.

The executive or main program calls this subroutine as it proceeds through the iterative scheme. The main program recognizes a reservoir exists in a node as it inspects the ISEQ array which contains the operation sequence of the node. A reservoir is designated with a zero in the ISEQ array.

The first call to the RESOPR subroutine in any time frame represents one of the three conditions in which the reservoir operation is simulated. During this first call, or condition one, the reservoir chemistry of the last time frame is stored in the array BEGRES. All releases made from the reservoir during the current time frame are made using the chemistry of the last time frame. The assumption is that of a complete chemistry mix through the reservoir will occur in a one-month time frame.

The sediment inflow from the last time frame is used to update the total sediment deposited in the reservoir and also to update the minimum capacity of the reservoir. It is obvious that this technique does not attempt to distribute the sediment deposited in any one month time frame on the basis of the fluctuating water surface levels.

Under condition one or the first call, it is assumed that all inflows to the system are transporting sediment in suspension; therefore, the total sediment inflow to be used in the next time frame updates are computed during the first call. The sediment inflow computation is made using the following expression:

$$Q_s = AQ_w^B$$

where Q_s = sediment inflow in tons per day;

Q_w = water inflow in cubic feet per second.

The coefficients A and B are predetermined from correlation studies made concerning the relationship of the sediment inflow rate and the water inflow rate. The sediment inflow rate is converted to volume as acre-feet per month using 75 pounds per cubic foot as the density of sediment (including voids). The computed volume of sediment is stored in array BEGRES for use in the next time frame.

The criteria for the operation of the reservoir during the first call or condition one is to store or release water from the reservoir so that the water surface level or reservoir capacity is as near as possible to the target levels or capacities as designated by the rule curve for the particular reservoir which is stored in the array RULE. The rule curve represents an ideal use of the reservoir holding capabilities for a one-year operation. Evacuations for flood control or maintaining certain reservoir levels for power requirements can also be accomplished with the use of the rule curve. An example rule curve is shown on Figure 18.

Constraints such as maximum or minimum release oftentimes prevent the attainment of the target levels or capacities during the first call to the reservoir for a particular time frame.

AN EXAMPLE RULE CURVE

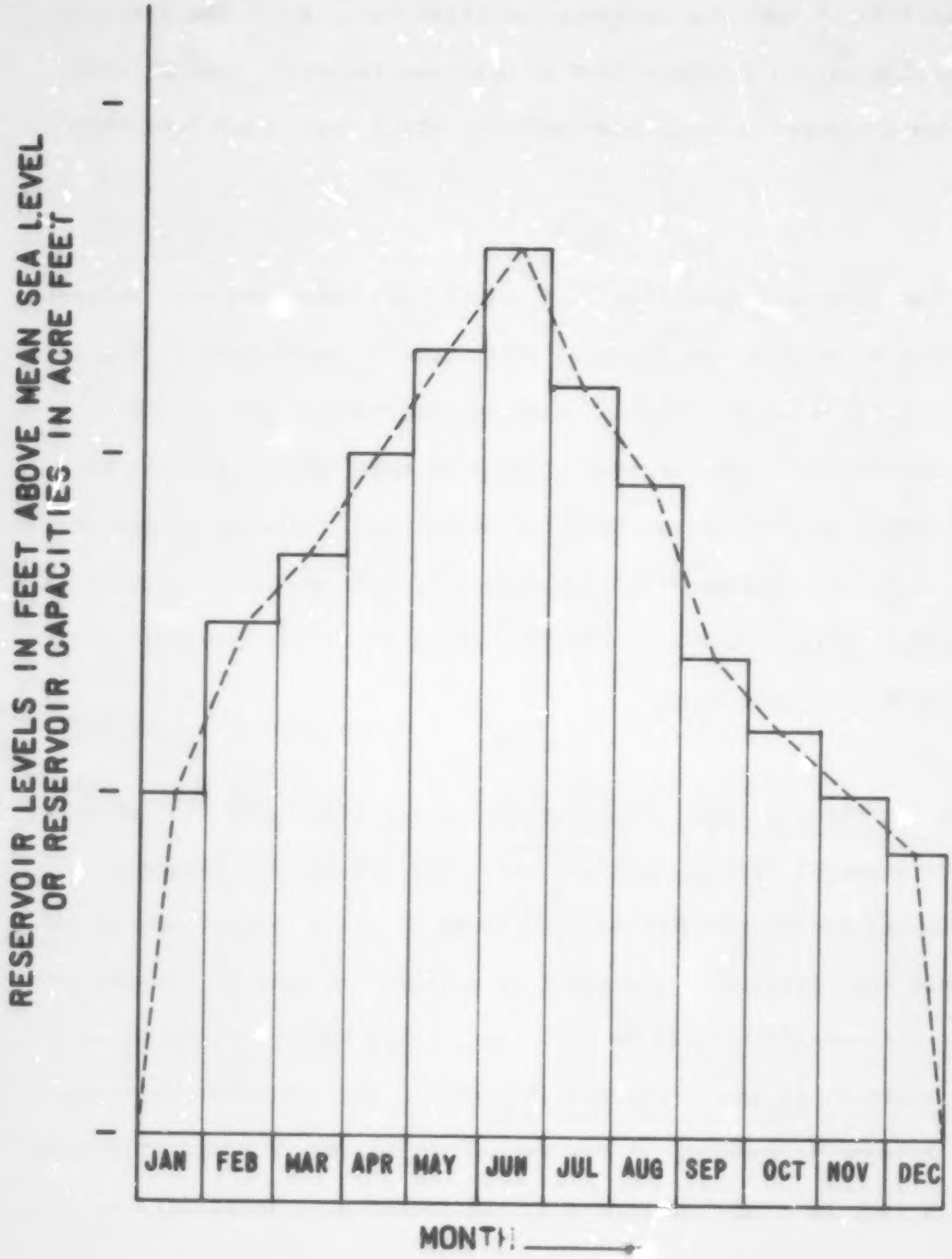


FIGURE 18

All other calls to the reservoir for a particular time frame are for the purpose of releasing water from the reservoir to meet a downstream deficit, which represents condition two, or for the purpose of passing waters released from an upstream reservoir through this reservoir to meet a downstream deficit, which represents condition three.

When the reservoir operation is simulated for condition two, releases are made to meet a downstream deficit. The releases made during this call are added to the releases made in the previous call. The constraints of maximum release or minimum capacity may prevent the reservoir from satisfying the total downstream requirement, and in such cases the maximum release possible is made and the reservoir is flagged to bypass further condition two calls to the reservoir during the particular time frame.

Condition three is the simulation of the reservoir operation where waters released from an upstream reservoir are passed through a particular reservoir which is downstream of the reservoir making the release and upstream of the point of deficit. A call to the reservoir under this condition will in most cases leave the reservoir in the same state as it was in the previous call. However, when the reservoir release is updated, it may exceed the maximum release constraint and in such an event the excess is considered as a spill for the purpose of continuity. It is possible that even though a spill is indicated, the reservoir level may not be high enough to utilize the spillway. An inspection of the reservoir level should be examined and the indicated spill may in effect become a reservoir bypass.

The reservoir chemistry at the end of the previous time frame is used as the chemistry of reservoir releases made during a particular time frame. The chemistry of the reservoir is continually updated for each and every inflow to the reservoir during a particular time frame.

Reservoir Evaporation

The evaporation losses from the reservoir water surface are in most cases the mean pan evaporation rates for the immediate locale of the reservoir. The mean rates are on a monthly basis and the variance from year to year is not considered significant. The evaporation rates as used by the model are in units of feet per acre of reservoir water surface area.

The monthly evaporation losses in units of acre-feet are computed by multiplying the mean reservoir water surface area by the evaporation rate for the particular month. In this respect, the model can easily be modified to include a more sophisticated simulation of evaporation losses as more information or better techniques become available. The mean water surface area is simply the mean of the area at the beginning of a time frame and that of the ith iteration.

The evaporation rates on a monthly basis are part of the model input data set and are stored in the array CONEVP for a 1-year period.

Reservoir Bank Storage

In some cases surface reservoirs have significant water absorption into the soils along the reservoir banks and in such cases this phenomenon is called "bank storage." As the reservoir level increases in elevation, the waters entering the bank are considered as additional reservoir storage. When the reservoir levels decrease in elevation, waters stored in the banks are released through capillary and/or other soil-water actions.

The simulation of this phenomenon is accomplished with the use of bank storage coefficients which are based upon experimental data and are stored on a monthly time frame in the array BANKCO. Consideration of "bank storage" is usually reserved for large reservoirs. The bank storage coefficient is multiplied by the change in storage (sign included) to determine the effects of "bank storage." A slight modification to this concept could be used to simulate reservoir seepage losses.

Capacity-Elevation Curves

The model simulates the physical water storage capacity of a surface reservoir with a series of second degree polynomials which are stored as base elevation and three coefficients in the RDATA array. The first derivative of these polynomials is used to compute the reservoir surface area. The polynomials relate reservoir capacity as a function of depth above the base elevation. The coefficients are determined from a stand alone computer program titled "CARCAP." However, any curve fitting mechanism would suffice and serve the same purpose.

An example of the capacity-elevation curve with an enlargement of the splines (ϵ) is shown on Figure 19. Twenty sets of second degree polynomials can be used to represent the capacity-elevation curve for the operating range of the surface reservoir. Discontinuities do exist between sets of polynomials; however, none are significant with respect to the general adequacy of the overall simulation.

General Information

The model is designed to take advantage of the high calculation speeds of the computer. Consequently, many iterations may be made through each node during any one time frame before whole river basin is balanced. All pertinent data arrays are updated both in volumes of water and chemistry of water at the end of each iteration. It follows then that several passes may be made through each reservoir in the river basin and each pass or iteration will update the RDATA array.

EXAMPLE CAPACITY-ELEVATION CURVE FOR SURFACE RESERVOIR

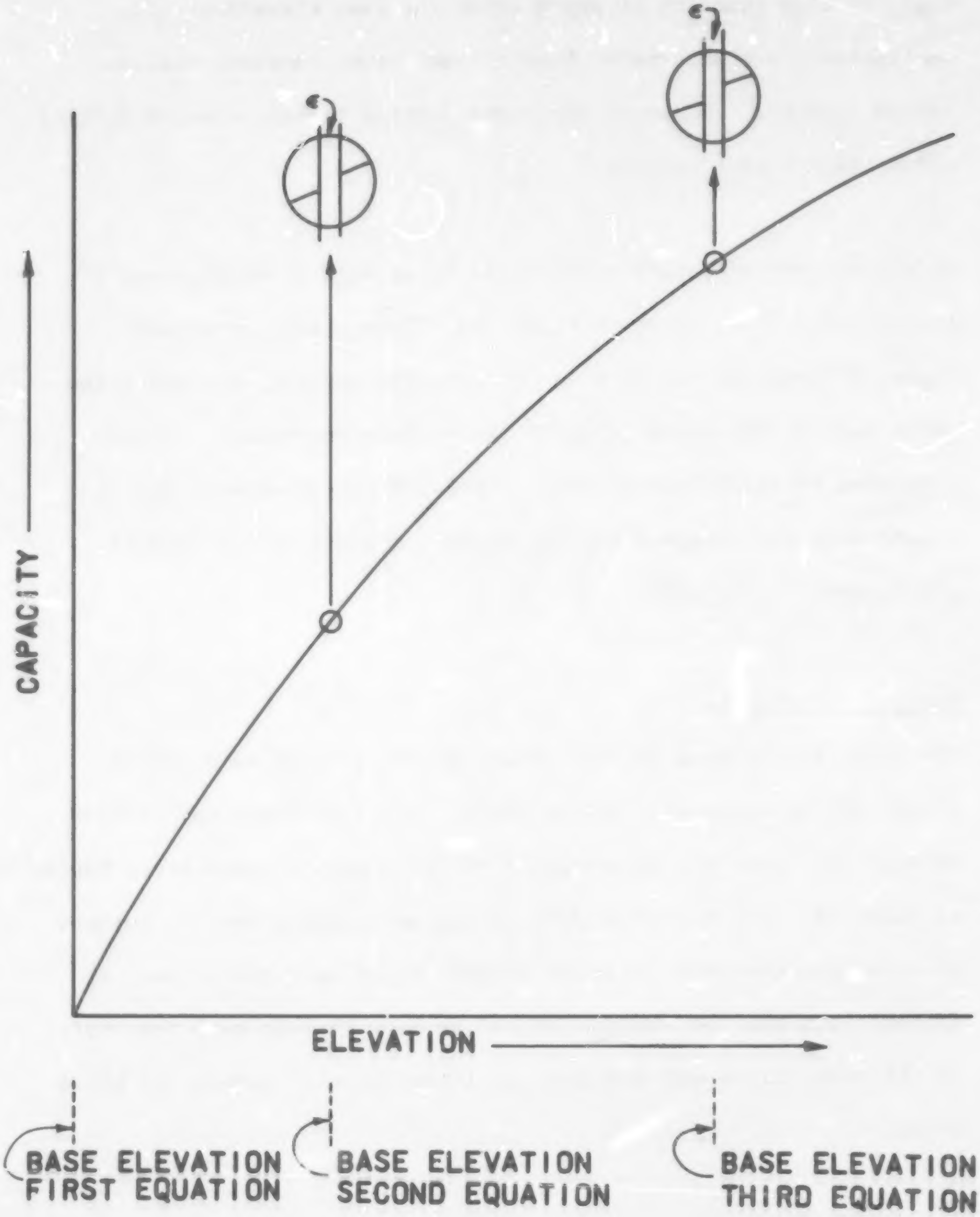


FIGURE 19

A call will be made to the subroutine PWROPR for each pass through a reservoir after the reservoir is in balance. In fact, the only route to subroutine PWROPR which simulates the operation of a powerplant is from subroutine RESOPR.

A general flow chart for the flow of the RESOPR subroutine is shown on Figures 20 through 22. The list of variable names and arrays is shown in Table 3.

FLOW CHART FOR SUBROUTINE RESOPR

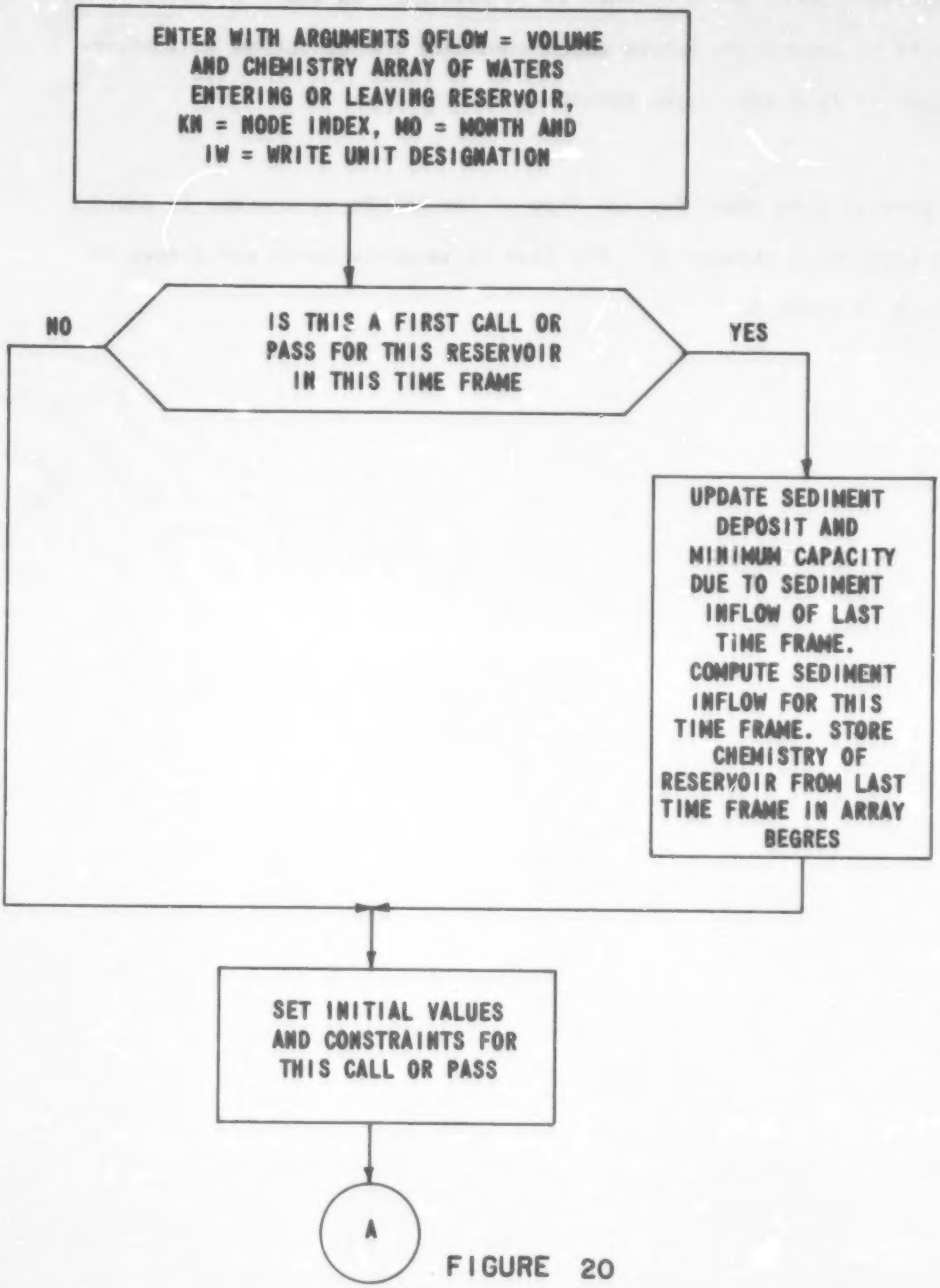

ENTER WITH ARGUMENTS QFLOW = VOLUME AND CHEMISTRY ARRAY OF WATERS ENTERING OR LEAVING RESERVOIR, KN = NODE INDEX, MO = MONTH AND IW = WRITE UNIT DESIGNATION
IS THIS A FIRST CALL OR PASS FOR THIS RESERVOIR IN THIS TIME FRAME
NO
YES
UPDATE SEDIMENT DEPOSIT AND MINIMUM CAPACITY DUE TO SEDIMENT INFLOW OF LAST TIME FRAME. COMPUTE SEDIMENT INFLOW FOR THIS TIME FRAME. STORE CHEMISTRY OF RESERVOIR FROM LAST TIME FRAME IN ARRAY BEGRES
SET INITIAL VALUES AND CONSTRAINTS FOR THIS CALL OR PASS
A

FIGURE 20

FLOW CHART FOR
SUBROUTINE RESOPR (CONT.)

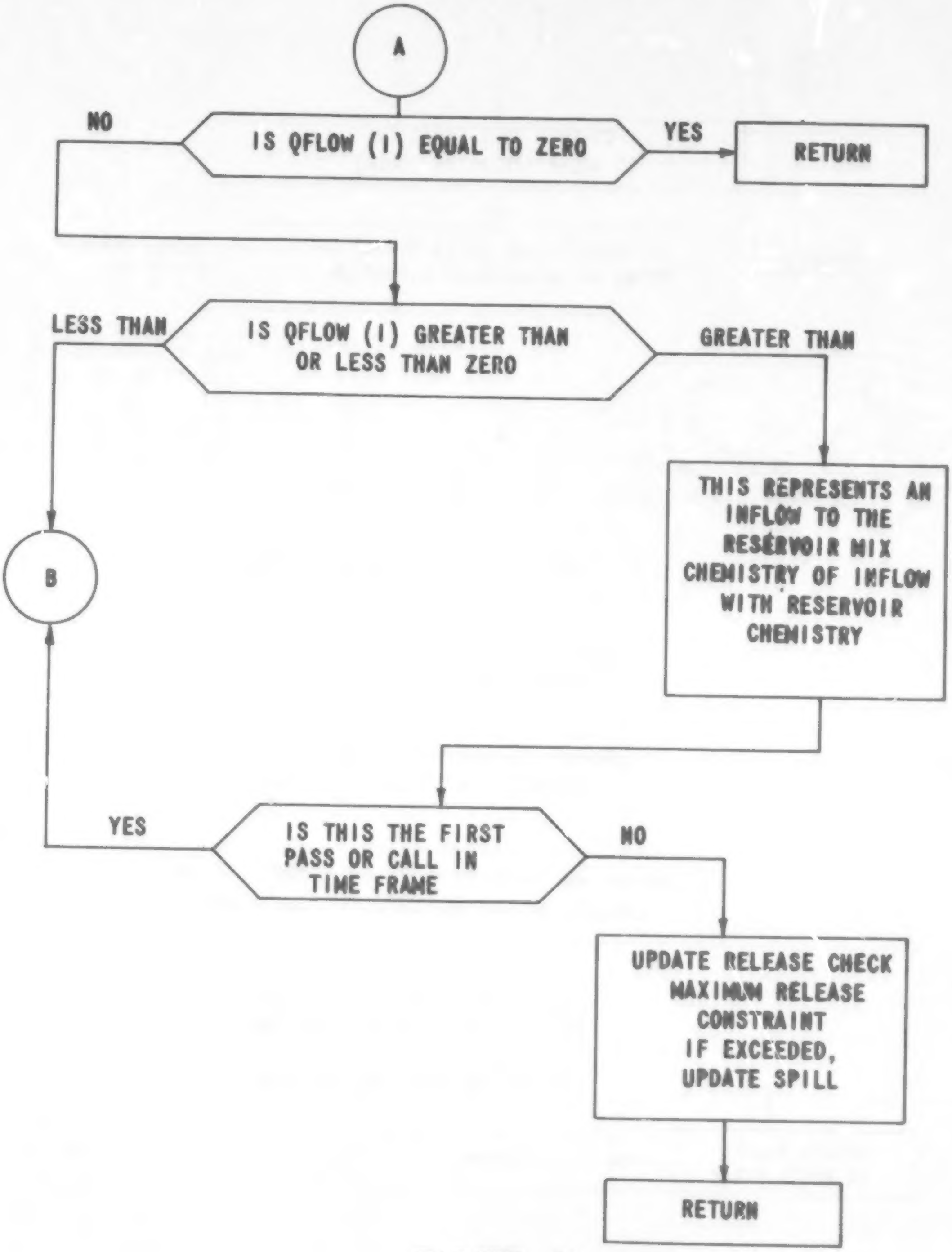

A
NO
IS QFLOW (I) EQUAL TO ZERO
YES
RETURN
LESS THAN
IS QFLOW (I) GREATER THAN OR LESS THAN ZERO
GREATER THAN
THIS REPRESENTS AN INFLOW TO THE RESERVOIR MIX CHEMISTRY OF INFLOW WITH RESERVOIR CHEMISTRY
B
YES
IS THIS THE FIRST PASS OR CALL IN TIME FRAME
NO
UPDATE RELEASE CHECK MAXIMUM RELEASE CONSTRAINT IF EXCEEDED, UPDATE SPILL
RETURN

FIGURE 21

FLOW CHART FOR SUBROUTINE RESOPR (CONT)

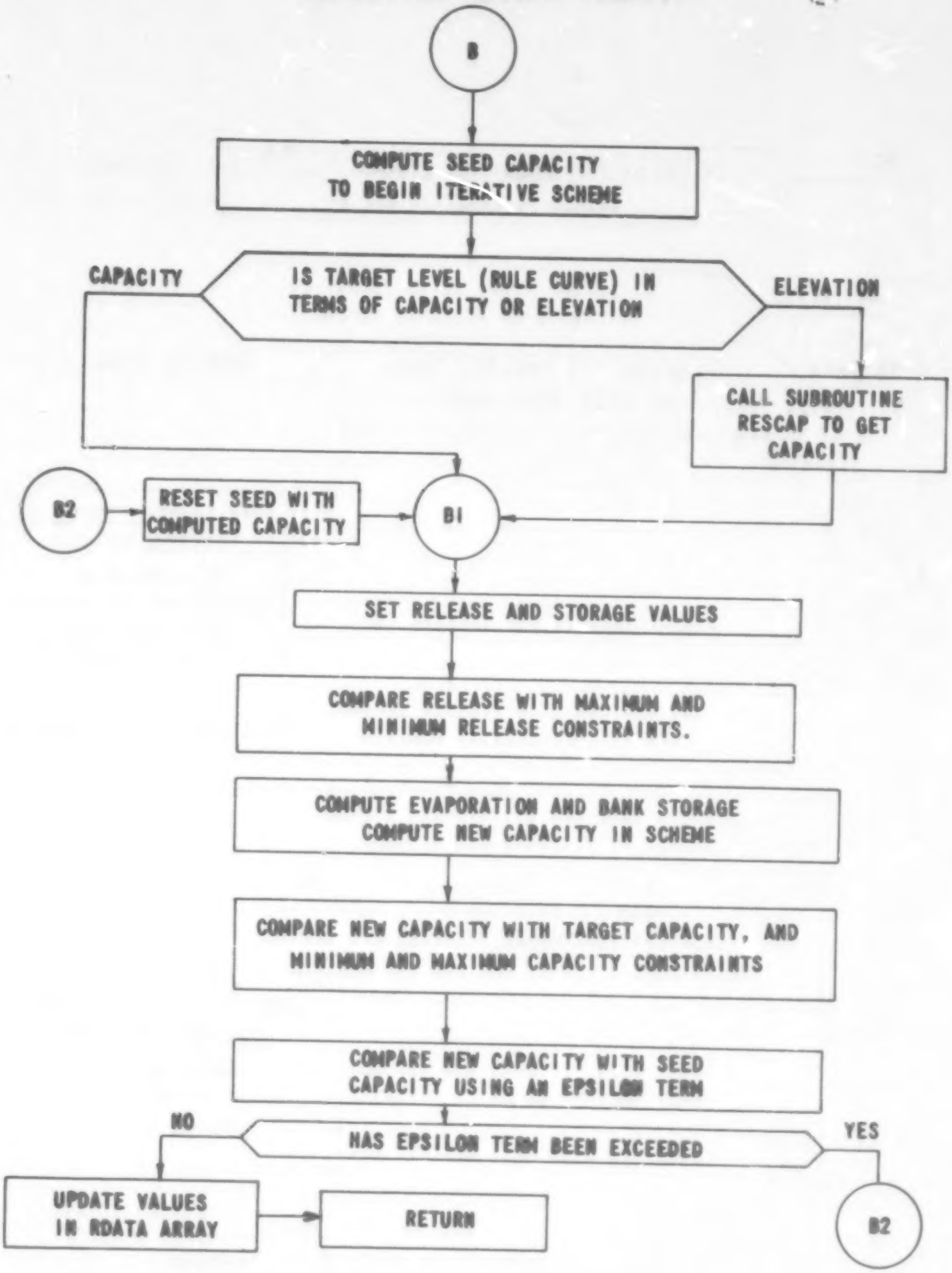

B
COMPUTE SEED CAPACITY TO BEGIN ITERATIVE SCHEME
CAPACITY
IS TARGET LEVEL (RULE CURVE) IN TERMS OF CAPACITY OR ELEVATION
ELEVATION
CALL SUBROUTINE RESCAP TO GET CAPACITY
B2
RESET SEED WITH COMPUTED CAPACITY
B1
SET RELEASE AND STORAGE VALUES
COMPARE RELEASE WITH MAXIMUM AND MINIMUM RELEASE CONSTRAINTS.
COMPUTE EVAPORATION AND BANK STORAGE COMPUTE NEW CAPACITY IN SCHEME
COMPARE NEW CAPACITY WITH TARGET CAPACITY, AND MINIMUM AND MAXIMUM CAPACITY CONSTRAINTS
COMPARE NEW CAPACITY WITH SEED CAPACITY USING AN EPSILON TERM
NO
HAS EPSILON TERM BEEN EXCEEDED
YES
UPDATE VALUES IN RDATA ARRAY
RETURN
B2

FIGURE 22

Table 3

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE RESOPR

Variable name	C*	Description	Remarks or units
AREA		Water surface area of reservoir	acres
A		First coefficient of sediment inflow equation	
BANKCO	C	Coefficient for use in "bank storage" computation	See data array BANKCO
BEGRES	C	Storage array for reservoir chemistry and sediment inflow at start of time frame	See data array BEGRES
B		Second coefficient of sediment inflow equation	
BSTOR		Bank storage value (with sign)	acre-feet
CAPBAB	C	Test used to determine if a power facility is part of reservoir complex	See data array CAPBAB in PWROPR subroutine
CAPMAX		Maximum capacity of reservoir	acre-feet
CAPMIN		Minimum capacity of reservoir	acre-feet
CAP		Computational aid for reservoir capacity	acre-feet
CAPX		Seed capacity in balancing reservoir water budget	acre-feet
CAPY		Check capacity used in iterative scheme to balance reservoir water budget	acre-feet
CHEMRR		Entry to subroutine CHEMGR	See subroutine CHEMGR

Table 3 - Continued

Variable name	C*	Description	Remarks or units
CONEVP		Evaporation rate for reservoir water surface area in feet per acre	See data array CONEVP
CONST		Conversion factor to convert feet cubed per second to acre-feet per day = 1.983471	
DAYS		Days in a particular month	
DELTAF		Additional release from a reservoir to meet a downstream deficit	acre-feet
DIFF		Absolute difference between seed (CAPX) and check capacity (CAPY)	acre-feet
ELEV		Reservoir water surface elevation	Feet above mean sea level
EPSLON		Term used to check convergence of reservoir balance = 10 acre-feet	
EVAP		Reservoir water surface evaporation	acre-feet
IDAYS		Data array with days of each month in a year - FEB = 28 days	
IFIR		Computational aid	
IMON		Month of calculation (particular time frame)	2 digits
IW		Write unit designation	
J		Loop index	
KA		Incremented loop index for storage in RDATA array	

Table 3 - Continued

Variable name	C*	Description	Remarks or units
KNODE		Node number	
KN		Part of argument list where KN = Node index	
K		Loop index	
MARK		Computational aid	
MODE		Computational aid	
MO		Month designation of particular time frame	
NCTRL		Node control array	See data array NCTRL
NITER		Iteration counter for scheme to balance reservoir water budget	
PREA		Reservoir water surface area of previous time frame	acres
PRECAP		Reservoir capacity of previous time frame	acre-feet
PREL		Reservoir water surface elevation of previous time frame	Feet above mean sea level
PWROPR		Enter to subroutine PWROPR	See subroutine PWROPR
QCFS		Inflow in cubic feet per second	Converted from acre-feet per month
QFLOW		Computational aid array used in various arguments	
QSED		Sediment inflow per time frame	acre-feet

Table 3 - Continued

Variable name	C*	Description	Remarks or units
RDATA		Array used to store surface reservoir parameters	See data array RDATA
RELAF		Reservoir release	acre-feet
RELCFS		Reservoir release	Cubic feet per second
RESCAP		Computational aid (reservoir capacity)	acre-feet
RESEL		Computational aid (Reservoir elevation)	Feet above mean sea level
RULE	C	Reservoir rule curve (Ideal operation levels on monthly basis)	See data array RULE
SPILL		Reservoir spill	acre-feet
STORAF		Reservoir storage per call or pass	acre-feet
TARGET		Target level (rule curve) as capacity	acre-feet
TEMCAP		Computational aid (reservoir capacity)	acre-feet

Table 3 - Continued

DATA ARRAYS IN SUBROUTINE RESOPR

DATA ARRAY BANKCO (20)

BANKCO (J) = Bank storage coefficient for reservoir in node "J" expressed as a decimal

J = Node index

DATA ARRAY BEGRES (20,11)

BEGRES (J,1) = Redundant (usually reserved for capacity of reservoir)

BEGRES (J,2) = Concentration of calcium in surface reservoir at beginning of time frame in ppm

BEGRES (J,3) = Concentration of magnesium

BEGRES (J,4) = Concentration of sodium

BEGRES (J,5) = Concentration of chloride

BEGRES (J,6) = Concentration of sulfate

BEGRES (J,7) = Concentration of bicarbonate

BEGRES (J,8) = Concentration of carbonate

BEGRES (J,9) = Concentration of nitrate

BEGRES (J,10) = Concentration of total salts (TDS)

BEGRES (J,11) = Sediment inflow for a particular time frame in acre-feet

J = Node sequence

DATA ARRAY RULE (20,13)

RULE (J,1) = Target level for January (Rule curve)

RULE (J,2) = Target level for February

Table 3 - Continued

DATA ARRAY RULE (20,13) - Continued

RULE (J,3) = Target level for March

RULE (J,4) = Target level for April

RULE (J,5) = Target level for May

RULE (J,6) = Target level for June

RULE (J,7) = Target level for July

RULE (J,8) = Target level for August

RULE (J,9) = Target level for September

RULE (J,10) = Target level for October

RULE (J,11) = Target level for November

RULE (J,12) = Target level for December

RULE (J,13) = Indicator of target level
0 = level in terms of capacity
1 = level in terms of elevation

J = Node index

DATA ARRAY RDATA (20,110)

RDATA (J,1) = Node number

RDATA (J,2) = Sequence number

RDATA (J,3) = Reservoir capacity at end of call in acre-feet

RDATA (J,4) = Reservoir water surface elevation at end of call in feet above mean sea level

RDATA (J,5) = Reservoir water surface area at end of call in acres

RDATA (J,6) = Reservoir evaporation loss at end of call in acre-feet

Table 3 - Continued

DATA ARRAY RDATA (20,110) - Continued

RDATA (J,7) = Reservoir change in bank storage in acre-feet (sign included) at end of call

RDATA (J,8) = Reservoir spill (spillway release) in acre-feet at end of call

RDATA (J,9) = Reservoir release through outlets and turbines in acre-feet at end of call

RDATA (J,10) = Total reservoir release - RDATA (J,8) + RDATA (J,9) in acre-feet at end of call

RDATA (J,11) = Maximum reservoir capacity in acre-feet

RDATA (J,12) = Minimum reservoir capacity in acre-feet

RDATA (J,13) = Maximum reservoir release (w/o spill) in cubic feet per second

RDATA (J,14) = Minimum reservoir release in cubic feet per second

RDATA (J,15) = "A_1" coefficient for equation - sediment = f (flow)

RDATA (J,16) = "B_1" coefficient for equation - sediment = f (flow)

RDATA (J,17) = "A_2" coefficient for equation - sediment = f (flow)

RDATA (J,18) = "B_2" coefficient for equation - sediment = f (flow)

RDATA (J,19) = Spline point for equations $Qs_1 = A_1Qw_1^{B_1}$ and $Qs_2 = A_2Qw_2^{B_2}$ in cubic feet per second - units on independent variable flow (Qw)

RDATA (J,20) = Total sediment in reservoir at start of time frame in acre-feet

RDATA (J,21-100) = Twenty base elevations plus coefficients for 20 second degree polynomials where - capacity = f (elevation increment)

Table 3 - Continued

DATA ARRAY RDATA (20,110) - Continued

RDATA (J,101) = Concentration of calcium in reservoir at end of call in ppm

RDATA (J,102) = Concentration of magnesium

RDATA (J,103) = Concentration of sodium

RDATA (J,104) = Concentration of chloride

RDATA (J,105) = Concentration of sulfate

RDATA (J,106) = Concentration of bicarbonate

RDATA (J,107) = Concentration of carbonate

RDATA (J,108) = Concentration of nitrate

RDATA (J,109) = Total salts (TDS) in ppm

RDATA (J,110) = Total salts (TDS) in tons per acre-feet

J = Node index

FUNCTION RESCAP

This function is used to determine the surface reservoir capacity when the reservoir water surface elevation is given. The reservoir surface elevation is passed as part of the argument along with the node index and write unit designation.

As mentioned earlier in this volume the reservoir capacity is a function of water surface elevation. This function is represented as a second degree polynomial and several polynomials may be used to describe this relationship from the minimum reservoir capacity to the maximum capacity or the operating pool of the reservoir.

The data required for each of these polynomials are stored in the RDATA array with four values entered for each polynomial. The first of these values is the base elevation pertaining to the particular polynomial, the second, third, and fourth values are the first, second, and third coefficients where the polynomial is represented in increasing powers of the independent variable.

An example of the RDATA array for the Steinaker Reservoir, which is a surface reservoir in the Vernal Project study, is shown in Table 4 .

Table 4

Pclynomials Used for Steinaker Reservoir

Base elevation	Coefficients First	 Second	 Third
5390 RDATA(KN,21)	0.0 RDATA(KN,22)	0.0 RDATA(KN,23)	0.05 RDATA(KN,24)
5400 RDATA(KN,25)	5.0 RDATA(KN,26)	1.0 RDATA(KN,27)	0.25 RDATA(KN,28)
5410 RDATA(KN,29)	40.0 RDATA(IN,30)	6.0 RDATA(KN,31)	2.00 RDATA(KN,32)
5420 RDATA(KN,33)	300.0 RDATA(KN,34)	46.0 RDATA(KN,35)	3.35 RDATA(KN,36)
5430 RDATA(KN,37)	1093.9286 RDATA(KN,38)	113.6071 RDATA(KN,39)	3.00 RDATA(KN,40)
5450 RDATA(KN,41)	4565.0 RDATA(KN,42)	233.0 RDATA(KN,43)	2.90 RDATA(KN,44)
5460 RDATA(KN,45)	7188.75 RDATA(KN,46)	288.875 RDATA(KN,47)	3.925 RDATA(KN,48)
5480 RDATA(KN,49)	14546.4286 RDATA(KN,50)	444.3571 RDATA(KN,51)	4.45 RDATA(KN,52)
5500 RDATA(KN,53)	25215.3175 RDATA(KN,54)	626.7523 RDATA(KN,55)	5.3717 RDATA(KN,56)

KN = Node index

An example can be made of the function with the use of the data shown in Table 4 . Given a reservoir water surface elevation = 5423.7 feet above mean sea level find the reservoir capacity that corresponds to this elevation.

A search is first made to find the first base elevation in the RDATA array that is greater than the given elevation. In this example that base elevation would be 5430.0. The location of this base elevation is decreased by four, i.e., RDATA(KN,37) to RDATA(KN,33) where the base elevation of 5420 is stored. The next three higher locations contain the coefficients of the required polynomials, i.e., RDATA(KN,34-36).

The reservoir capacity would be computed as follows:

Let: $h = 5423.7 - 5420.0 = 3.7$ feet

then: $\text{capacity} = 300.0 + 46.0\ (3.7) + 3.35\ (3.7)(3.7) = 516$ acre-ft

The above example is offered in lieu of a flow chart. The variable names are self-explanatory and the data arrays have been previously explained.

FUNCTION RESEL

This function is the converse of Function RESCAP where the reservoir capacity is given, and it is necessary to find the reservoir water surface elevation for the given capacity.

The argument list includes the capacity, reservoir water surface area, node index, and write unit designation.

The reservoir elevation is determined by the solution of a quadratic equation once the proper set of coefficients has been found for the particular capacity. The first coefficient of the second degree polynomial is actually the capacity at the particular base elevation.

The reservoir water surface area for the given capacity is determined by solving for the derivative dc/dh.

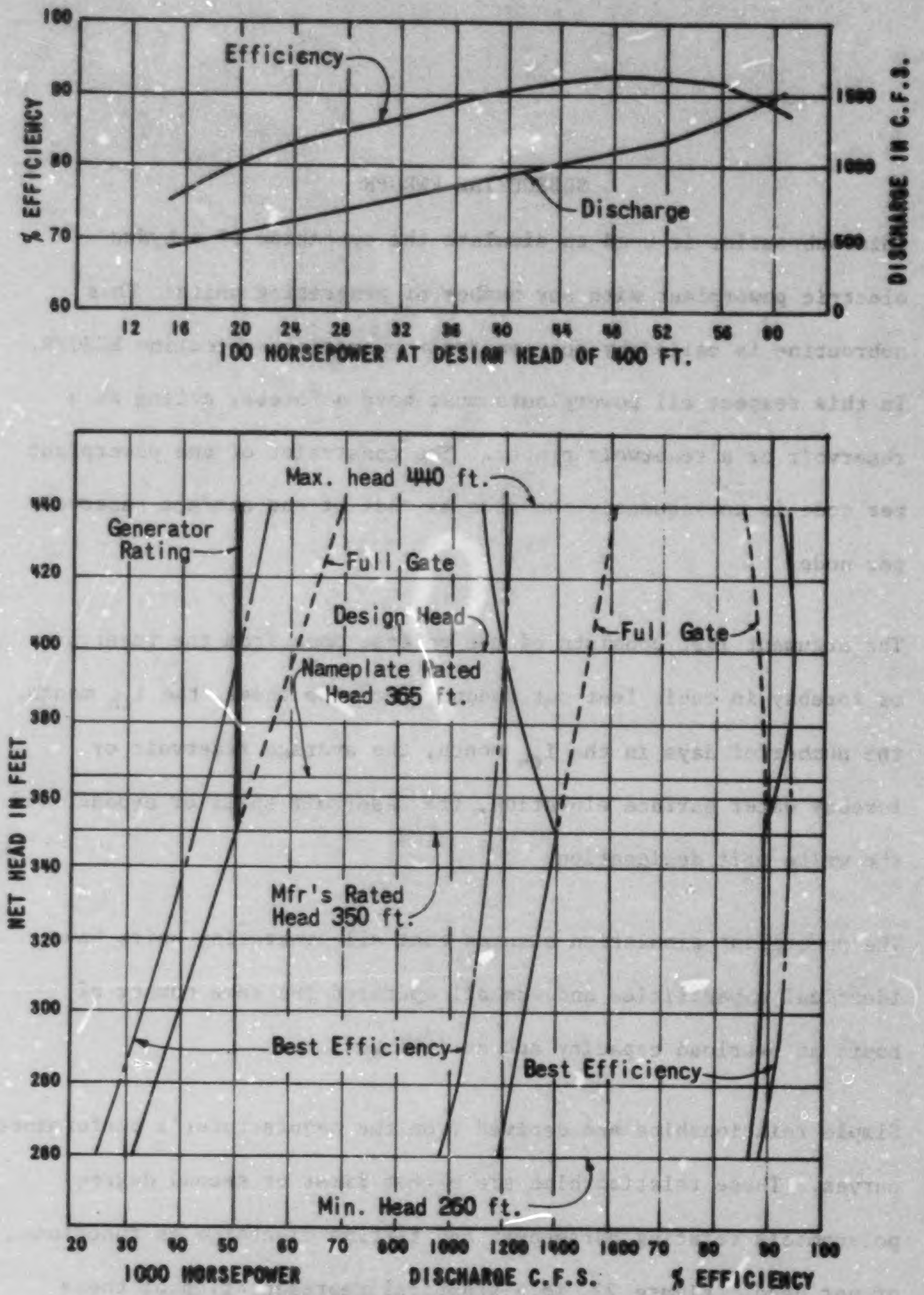
SUBROUTINE PWROPR

This subroutine is used to simulate the operation of a hydroelectric powerplant with any number of generating units. This subroutine is called by the reservoir operation subroutine RESOPR. In this respect all powerplants must have a forebay acting as a reservoir or a reservoir proper. The constraint of one powerplant per node is consequently the same as that of one surface reservoir per node.

The argument list consists of the release made from the reservoir or forebay in cubic feet per second, the node index, the i_{th} month, the number of days in the i_{th} month, the average reservoir or forebay water surface elevation, the reservoir spill or bypass, and the write unit designation.

The powerplant simulation assumes that all generating units have identical capabilities and are all operated the same number of hours at overload capacity and at full gate.

Simple relationships are derived from the manufacturer's performance curves. These relationships are either first or second degree polynomials relating horsepower and turbine discharge as functions of net head. Figure 23 is a graphical representation of these relationships. Consideration has been given to an optimum



SAMPLE PREDICTED CHARACTERISTIC CURVES

FIGURE 23

combination of operating at best gate and full gate as the net head varies. However, when simulating with a 1-month time frame and the assumptions necessary for other pertinent variables made this consideration an invalid refinement.

Efficiency is computed as the ratio of actual horsepower to the theoretical horsepower when the net head is less than the head of maximum discharge. When the net head is equal to or greater than the head at maximum discharge a constant efficiency is used.

The tailwater elevation is computed by entering a polynomial with total discharge in cubic feet per second as the independent variable. Coefficients for this polynomial are stored in the TDATA array.

The net head is simply the average reservoir water surface elevation minus the tailwater elevation. Other minor head losses can easily be inserted (if known) into the simulation with a slight modification to the subroutine.

A firm power demand curve can be included at each powerplant site. This curve is represented as kilowatt-hours per month. The curve is assumed not to change from year to year; however, if changes are desired they can be inserted with the use of transaction cards. The curve is stored in the data array PDATA. A sample of a firm power demand curve is shown on Figure 24. This type of curves can be used to provide a desired distribution of a system power demand. In this version of the powerplant simulation no provision is made to increase reservoir or forebay release if power generated is less than firm demand (iterative procedure) or to halt computation if firm demand is not met. All power generated greater than firm demand is considered as secondary power.

An iterative scheme is used in determining power generation as the tailwater elevation and therefore the net head changes per iteration. The epsilon term in the iterative scheme is the flow through the turbines and is presently set at 5 cubic feet per second.

The number of hours of operation is determined as the ratio of total water released from the reservoir to the total water released through the turbines multiplied by the number of hours in the particular month. Whenever this ratio is greater than 1.0 it is set to 1.0 and the difference between the water released through the turbines and the total water released from the reservoir is assumed to be released through the outlet works.

All power generated is computed in units of kilowatt-hours.

A general flow chart for this subroutine is shown on Figures 25 and 26 and the list of variable names and arrays is shown in Table 5 .

AN EXAMPLE POWER DEMAND CURVE

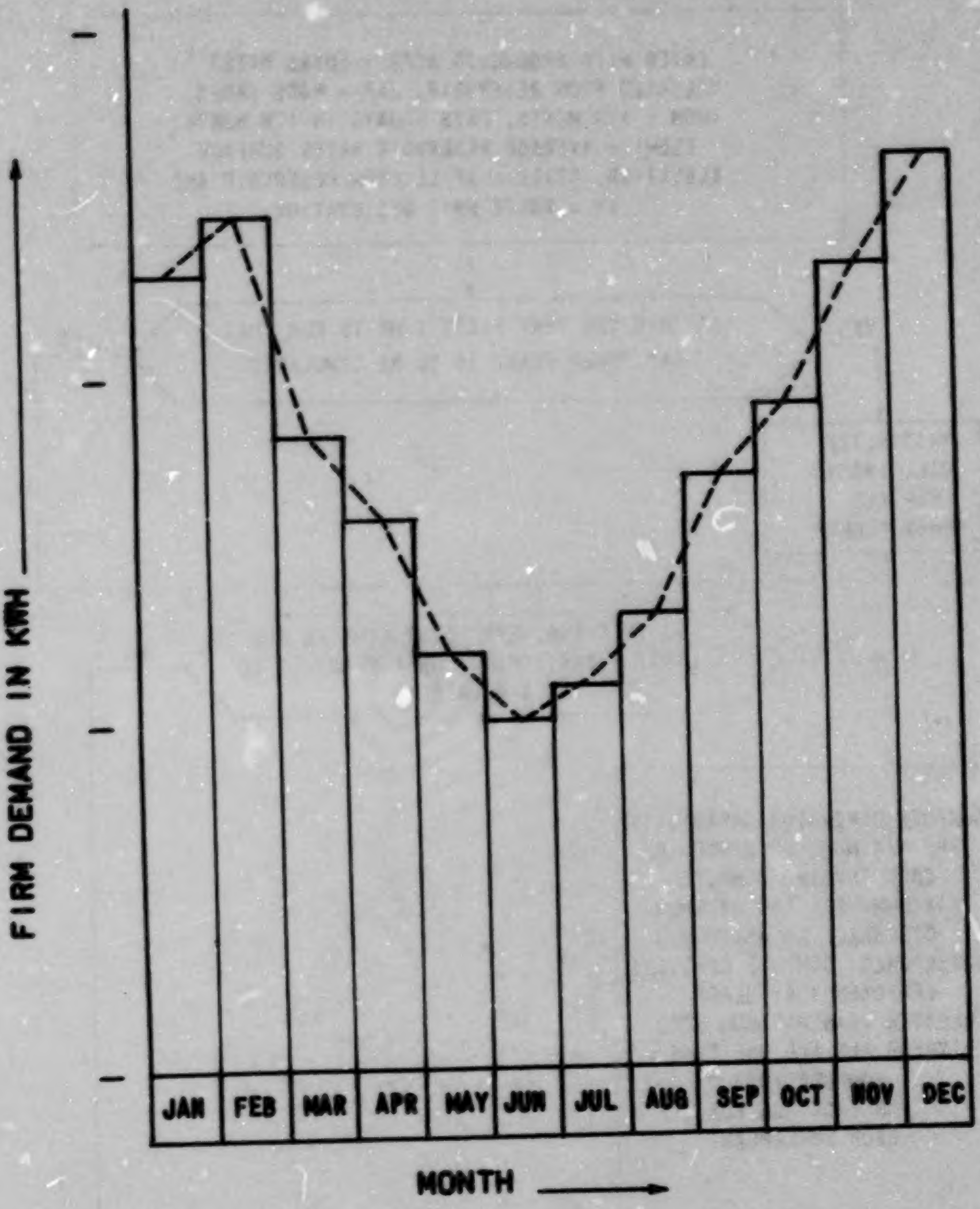


FIGURE 24

FLOW CHART FOR SUBROUTINE PWROPR

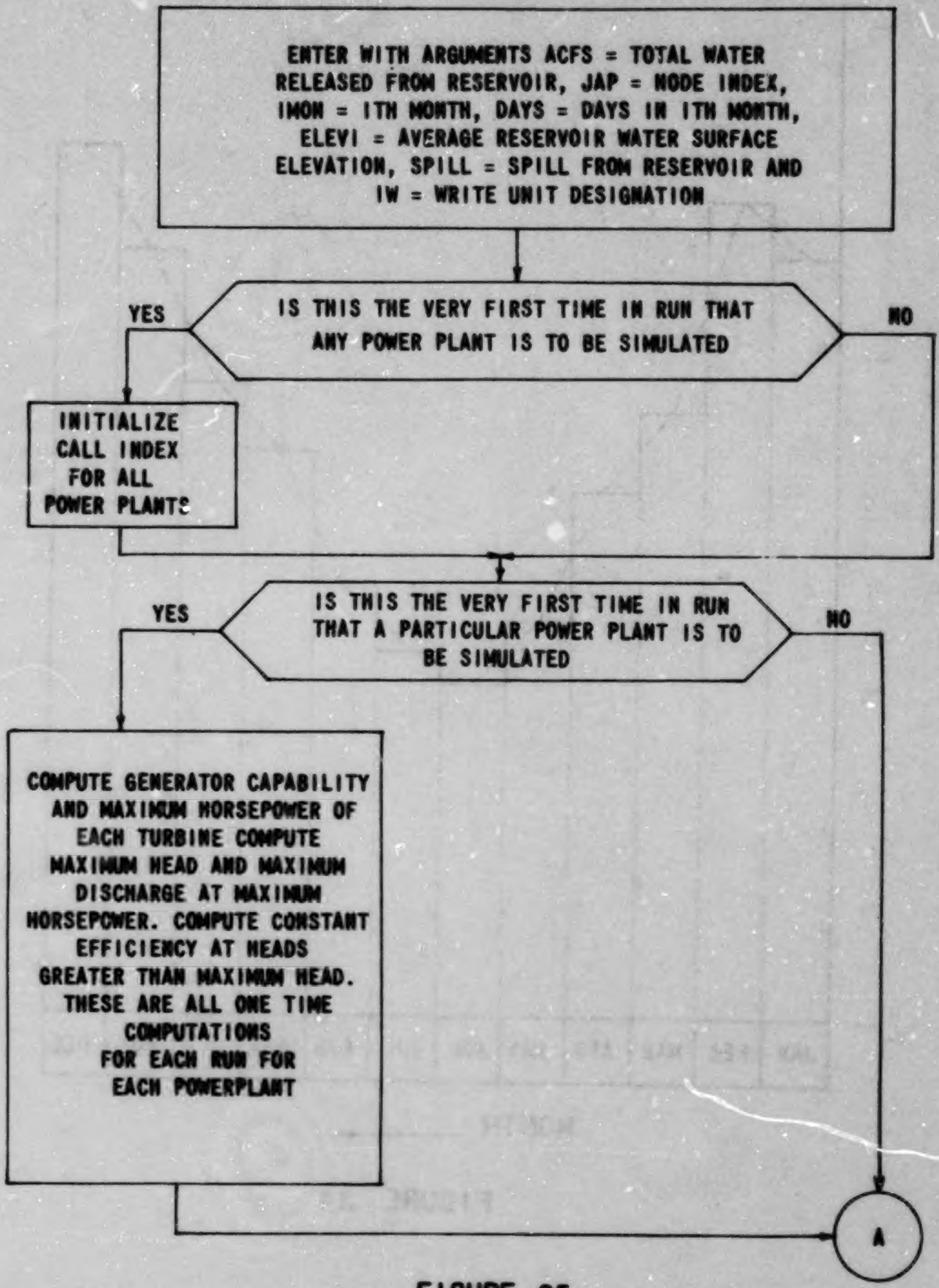
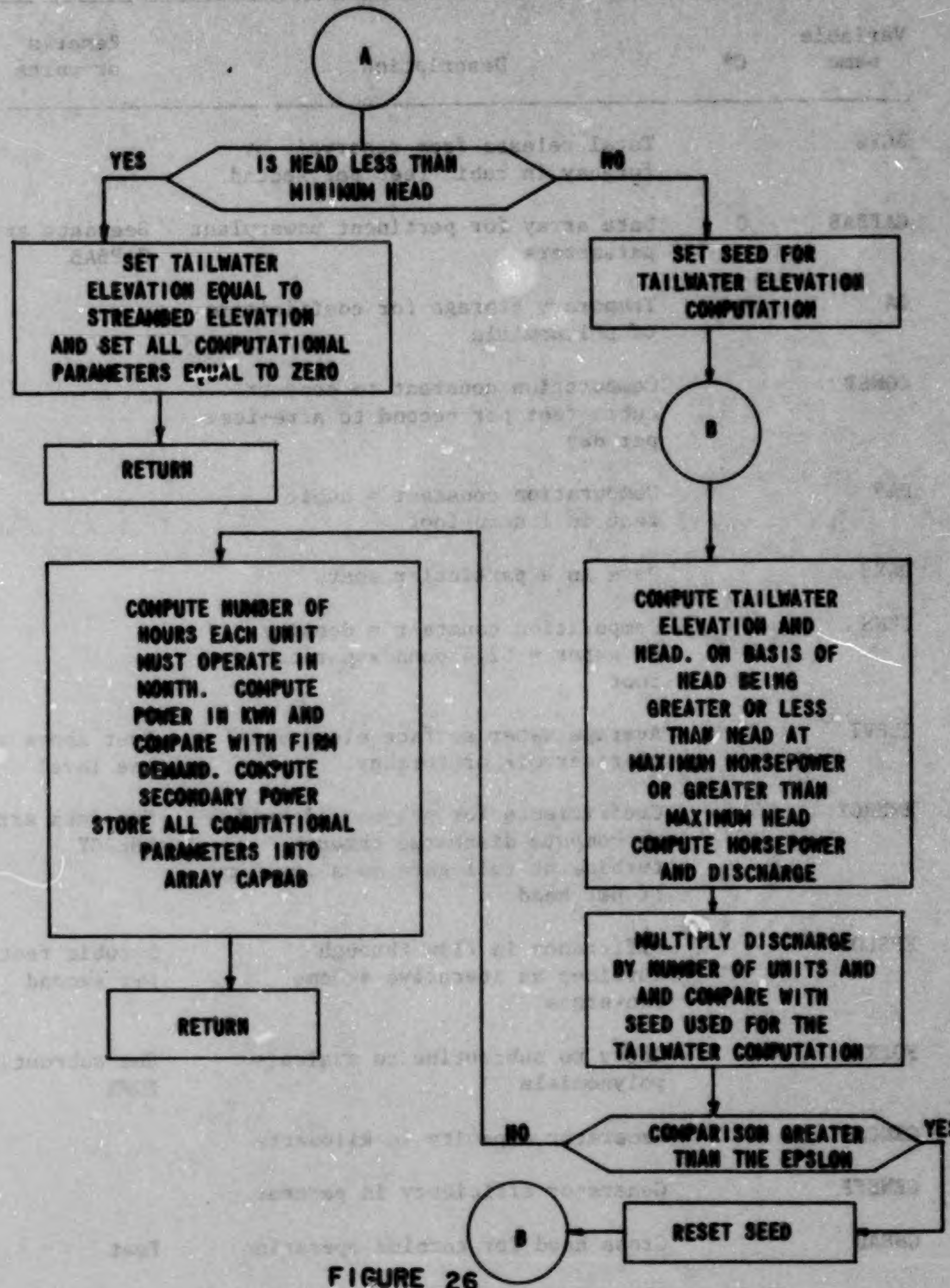

ENTER WITH ARGUMENTS ACFS = TOTAL WATER RELEASED FROM RESERVOIR, JAP = NODE INDEX, IMON = ITH MONTH, DAYS = DAYS IN ITH MONTH, ELEVI = AVERAGE RESERVOIR WATER SURFACE ELEVATION, SPILL = SPILL FROM RESERVOIR AND IW = WRITE UNIT DESIGNATION
IS THIS THE VERY FIRST TIME IN RUN THAT ANY POWER PLANT IS TO BE SIMULATED
YES
NO
INITIALIZE CALL INDEX FOR ALL POWER PLANTS
IS THIS THE VERY FIRST TIME IN RUN THAT A PARTICULAR POWER PLANT IS TO BE SIMULATED
YES
NO
COMPUTE GENERATOR CAPABILITY AND MAXIMUM HORSEPOWER OF EACH TURBINE COMPUTE MAXIMUM HEAD AND MAXIMUM DISCHARGE AT MAXIMUM HORSEPOWER. COMPUTE CONSTANT EFFICIENCY AT HEADS GREATER THAN MAXIMUM HEAD. THESE ARE ALL ONE TIME COMPUTATIONS FOR EACH RUN FOR EACH POWERPLANT
A

FIGURE 25

FLOW CHART FOR
SUBROUTINE PWROPR (CONT.)



A
IS HEAD LESS THAN MINIMUM HEAD
YES
NO
SET TAILWATER ELEVATION EQUAL TO STREAMBED ELEVATION AND SET ALL COMPUTATIONAL PARAMETERS EQUAL TO ZERO
RETURN
SET SEED FOR TAILWATER ELEVATION COMPUTATION
B
COMPUTE TAILWATER ELEVATION AND HEAD. ON BASIS OF HEAD BEING GREATER OR LESS THAN HEAD AT MAXIMUM HORSEPOWER OR GREATER THAN MAXIMUM HEAD COMPUTE HORSEPOWER AND DISCHARGE
MULTIPLY DISCHARGE BY NUMBER OF UNITS AND AND COMPARE WITH SEED USED FOR THE TAILWATER COMPUTATION
COMPARISON GREATER THAN THE EPSLON
NO
YES
RESET SEED
B
COMPUTE NUMBER OF HOURS EACH UNIT MUST OPERATE IN MONTH. COMPUTE POWER IN KWH AND COMPARE WITH FIRM DEMAND. COMPUTE SECONDARY POWER STORE ALL COMUTATIONAL PARAMETERS INTO ARRAY CAPBAB
RETURN

FIGURE 26

Table 5

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE PWROPR

Variable name	C*	Description	Remarks or units
ACFS		Total release from reservoir or forebay in cubic feet per second	
CAPBAB	C	Data array for pertinent powerplant parameters	See data array CAPBAB
CA		Temporary storage for coefficients of polynomials	
CONST		Computation constant to convert cubic feet per second to acre-feet per day	
DAF		Computation constant = cubic feet in 1 acre-foot	
DAYS		Days in a particular month	
DENS		Computation constant = density of water = 62.4 pounds per cubic foot	
ELEVI		Average water surface elevation of reservoir or forebay	Feet above mean sea level
ENERGY	C	Coefficients for polynomial used to compute discharge through turbine at full gate as a function of net head	See data array ENERGY
EPSLON		Difference in flow through turbines as iterative scheme converges	5 cubic feet per second
FOFX		Entry to subroutine to evaluate polynomials	See subroutine FOFX
GENCAP		Generator capacity in kilowatts	
GENEFF		Generator efficiency in percent	
GHEAD		Gross head for turbine operation	Feet

Table 5 - Continued

Variable name	C*	Description	Remarks or units
HDMAX		Maximum head for turbine operation	Feet
HDMIN		Minimum head for turbine operation	Feet
HOURS		Hours of operation for each turbine	
HPF		Computation constant to convert foot-pounds per second to horsepower	
HPMAX		Maximum horsepower for turbine operation	
HPTOKW		Computation constant to convert horsepower to kilowatts	
IFIR		Computation index designating entry sequence to subroutine	
IMON		Month designation of particular time frame	
IW		Write unit designation	
JAP		Node index	
KA		Loop index	
KNODE		Node number	
KP		Node index in loop	
K		Loop index	
KSET		Computation index of head with respect to head at maximum horsepower or at maximum head	
KWH		Power generation for all units combined in kilowatt-hours	
KWHSEC		Secondary or dump power generated for all units combined in kilowatt-hours	

Table 5 - Continued

Variable name	C*	Description	Remarks or units
MODE		Computational index used for each iteration into subroutine for each node	
MOLE		Alpha designation of source of call in obtaining root of equations	See subroutine ROOTWO
NCTRL	C	Control array - See previous definition of this array	
PDATA	C	Data array containing firm power requirements on a monthly basis	See data array PDATA
RATIO		Ratio of total discharge released from reservoir to total discharge through all turbines combined	
RCFS		Second guess in iterative scheme for power generated per unit in cubic feet per second	
RELAF		Discharge through all turbines combined in acre-feet	
RKWH		Firm power demand for particular month in kilowatt-hours	
ROOTWO		Entry into subroutine to determine root of polynomial	See subroutine ROOTWO
SPILL		Reservoir release not passed through turbines or outlet works	Acre-feet
TCFS		Discharge through turbine at maximum horsepower in cubic feet per second	Full gate
TDATA		Coefficients for polynomial describing tailwater elevation as a function of discharge through turbines and outlet works in cubic feet per second	See data array TDATA

Table 5 - Continued

Variable name	C*	Description	Remarks or units
TEFF		Turbine efficiency in percent	
TEST		Computational aid = average reservoir water surface elevation minus streambed elevation	Feet
THEAD		Head at maximum horsepower	Feet
THEORY		Computational aid representing turbine horsepower assuming 100 percent effiency	
THP		Computed horsepower of turbine from solution of polynomial - where horsepower is a function of net head	
TKW		Computation aid representing kilowatts generated per unit	
TOTCFS		Total discharge through all turbines combined in powerplant in cubic feet per second	
TOTKW		Total generation of all units combined in powerplant in kilowatts	
TSPILL		Reservoir spill or bypass in units of cubic feet per second. Used only when spillway or bypass unit discharge affects tailwater	
TWEL		Tailwater elevation	Feet above mean sea level
UNITS		Number of units in powerplant, i.e., turbines and generators	
XT		Independent variable representing total discharge in cubic feet per second in polynomial where tailwater elevation is a function of XT	

Table 5 - Continued

DATA ARRAYS IN SUBROUTINE PWROPR

DATA ARRAY ENERGY (20,8)

This data array contains the coefficients for the polynomial where turbine discharge is a function of net head in the first four locations, i.e., ENERGY (J,1-4). The polynomial is as follows:

Discharge = $A_1 + A_2H + A_3h^2 + A_4h^3$, where h = net head in feet. Then:

ENERGY (J,1) = A_1

ENERGY (J,2) = A_2

ENERGY (J,3) = A_3

ENERGY (J,4) = A_4

The second portion of the data array, i.e., ENERGY (J,5-8) contains the coefficients for the polynomial where turbine horsepower is a function of net head. The polynomial is as follows:

Horsepower = $A_1 + A_2h + A3h^2 + A_4h^3$, where h = net head in feet. Then

ENERGY (J,5) = A_1

ENERGY (J,6) = A_2

ENERGY (J,7) = A_3

ENERGY (J,8) = A_4

J = Node index

Table 5 - Continued

DATA ARRAY TDATA (20,4)

This data array contains the coefficients for the polynomial where tailwater elevation* is a function of total discharge through powerplant and/or outlet works in cubic feet per second. The polynomial is as follows: Tailwater elevation = $A_1 + A_2Q + A_3Q^2 + A_4Q^3$, where Q = discharge in cubic feet per second. Then:

TDATA (J,1) = A_1 (streambed elevation)

TDATA (J,2) = A_2

TDATA (J,3) = A_3

TDATA (J,4) = A_4

J = Node index

* Tailwater elevation is feet above mean sea level

DATA ARRAY PDATA (20,12)

PDATA (J,1) = Firm power demand in kilowatt-hours for January

PDATA (J,2) = Firm power demand for February

PDATA (J,3) = Firm power demand for March

PDATA (J,4) = Firm power demand for April

PDATA (J,5) = Firm power demand for May

PDATA (J,6) = Firm power demand for June

PDATA (J,7) = Firm power demand for July

PDATA (J,8) = Firm power demand for August

PDATA (J,9) = Firm power demand for September

Table 5 - Continued

DATA ARRAY PDATA (20,12) Continued

PDATA (J,10) = Firm power demand for October

PDATA (J,11) = Firm power demand for November

PDATA (J,12) = Firm power demand for December

J = Node index

DATA ARRAY CAPBAB (20,20)

CAPBAB (J,1) = Number of units (turbines) in powerplant

CAPBAB (J,2) = Generator rating in kva

CAPBAB (J,3) = Power factor (dimensionless)

CAPBAB (J,4) = Percent overload allowed each generator

CAPBAB (J,5) = Generator capability in kilowatts

CAPBAB (J,6) = Generator efficiency in percent

CAPBAB (J,7) = Maximum net head in feet

CAPBAB (J,8) = Minimum net head in feet

CAPBAB (J,9) = Maximum horsepower of turbine at overload

CAPBAB (J,10) = Head at maximum horsepower (full gate) in feet

CAPBAB (J,11) = Discharge through turbine at maximum horsepower in cubic feet per second

CAPBAB (J,12) = Turbine efficiency at maximum horsepower in percent

CAPBAB (J,13) = Hours in month each turbine operates at overload

CAPBAB (J,14) = Total power from powerplant for month in kilowatt-hours

Table 5 - Continued

DATA ARRAY CAPBAB (20,20) Continued

CAPBAB (J,15) = Total discharge through all units in acre-feet

CAPBAB (J,16) = Tailwater elevation in feet above mean sea level

CAPBAB (J,17) = Gross head (same as net head) in feet

CAPBAB (J,18) = Firm power generated in kilowatt-hours

CAPBAB (J,19) = Secondary or dump power generated in kilowatt-hours

CAPBAB (J,20) = Actual turbine efficiency in percent

J = Node index

SUBROUTINE DTABLE

This subroutine is used to rank all the reservoirs within the river basin for use in the determination of which reservoir should be called first, second, third, etc., on the basis of the least loss in elevation with the greatest incremental change in capacity. Ranking in this manner is for the purpose of maintaining the maximum net head for power generation.

When the ranking is completed the reservoirs are called in the resulting sequence to satisfy a deficit in meeting a downstream requirement. It is obvious that only reservoirs that are accessible and upstream of a deficit will be ranked in the calling sequence. The sequence in considering each node in the river basin, i.e., beginning with node farthest upstream and the operational node of the simulation, will insure that none of the deficit calls to a particular reservoir represents a first call to the reservoir.

Recalling the use of second degree polynomials to relate reservoir capacity (dependent variable) to the reservoir water surface elevation and delta increments of elevation (independent variable), it can easily be shown that the first derivative ($^{dc}/dh$) is the reservoir water surface area. Consequently, the reservoir with the largest water surface area will have the highest rank.

This subroutine in effect is a means of selecting withdrawals from the various surface reservoirs or a decision table for the operation of the reservoirs within the river basin.

Other factors may be considered in designing a decision table such as that described for this subroutine; however, the logic used in this subroutine has proven to be satisfactory for most river basin simulations. In any event the task of modifying the logic would be very simple if some other criteria were desired in setting a sequence of ranking reservoirs for the purpose of selective withdrawals. The variable names and arrays are shown in Table 6.

The argument list includes the node index, an array for the storage of node numbers of nodes containing reservoirs upstream and accessible to meet a deficit in a downstream node in a ranked sequence, an index of the number of upstream reservoirs that can be used to meet the deficit, and the number of operational sequences in the node where the deficit exists.

Table 6

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE DTABLE

Variable name	C*	Description	Remarks or units
AREA		Water surface area of reservoir in acres	
IC		Index used as an indicator of number of upstream reservoirs	
ISEQ	C	Operational sequence array for each node	See previous definition of this array (page 62)
KFA		Storage array of node numbers of nodes upstream and accessible to meet deficit	
KN		Node index of upstream node	
K		Loop index	
KS		Index of number of operation sequences in node of deficit	
LTEMP		Computational aid	
MAX		Computational aid used in ranking technique (maximum)	
MIN		Computational aid used in ranking technique (minimum)	
NCTRL		Control array for the simulation sequence of a river basin	See previous definition of this array (page 60)
NDWTR		Control array for the simulation sequence of a river basin	See previous definition of this array (page 62)
NFIND		Entry to subroutine NFIND	See subroutine NFIND

Table 6 - Continued

Variable name	C*	Description	Remarks or units
RDATA	C	Array used to store reservoir data	See previous definition of this array (Table 3)
TEMP		Computational aid	

ARRAY AREA (20) = Temporary storage array for reservoir areas upstream and accessible to meet downstream deficit

ARRAY KFA (20) = Storage array of node numbers of ranked reservoirs in descending order of reservoir areas

The dimension (20) represents the maximum number of nodes that can be used in simulation model.

FUNCTION NFIND

This function provides a simple method of determining the operational sequence of a node in the river basin. The argument list contains only the node number. A search is made of the node control array NCTRL to find the operational sequence of the node.

The need to find the operational sequence of the node occurs several times in the simulation model; therefore, this simple function is well justified.

SUBROUTINE RFCOMP

This subroutine is among the most essential of all techniques used in the simulation. It is primarily designed to simulate the magnitude and chemistry of return flow from either an irrigation or municipal and industrial demand (diversion). The subroutine also provides the mechanism to simulate exchanges of flow and chemistry that must exist between surface and subsurface facilities to maintain a hydraulic balance in each node.

An earlier version of this subroutine was more complex requiring greater quantities of data and containing several more empirical relationships in an attempt to define in a rigorous manner the deposition and timing (lagging) of the excess or return flow. Many applications were made using this early version, and it was concluded that uncertainties concerning the deposition and timing of returnable flows were often the result of lack of adequate data and, in some part, lack of technology. Consequently, much of the sophistication of the earlier version was discarded in favor of the simpler approach as contained in this subroutine where the exchange mechanism was adopted to "black box" many of the uncertainties and not destroy the validity of the simulation.

The argument list includes an array where magnitude and chemistry are stored for either incoming or outgoing waters, the node index, the operational sequence in the node, an index signifying the type computation to be performed by the subroutine, the i_{th} month, a constant, and the write unit designation.

The application of the simulation model is highly dependent upon an accurate determination of the types of uses of the water resources and the deposition of the excess or return flow. A use as defined in this simulation model is that water that is actually consumed to support plant or animal life (in effect leaves the system or river basin). An industrial requirement may or may not be considered a use by this definition.

The supply of an irrigation or municipal and industrial need begins with a point of diversion on a river, stream, or main service canal. This diversion is transported by means of smaller canals either lined or unlined to a farm area, municipality, or industrial site. As these waters are being transported, losses occur by evaporation and seepage into the soils of the unlined conveyances. Further losses occur after the waters reach the farm area by seepage losses of unlined laterals and by irrigating crops (plants) in excess of their needs. Additional losses and excesses are also experienced after waters reach a municipality. Most of the municipal losses are collected in a sewer system and treated before returning to the river basin. Simulation of the treatment facilities of these municipal losses has not been included in this version of the model; however, such a simulation is easily incorporated into the model if flow through rates and types of treatment are known.

The preceding brief background information has been included in this narrative to aid the user in understanding some of the philosophy used in the design of this subroutine.

Consumptive Use

The consumptive use as treated in this subroutine is actually that amount of water that leaves the river basin either in support of plant life (crops) or in support of a municipality or industrial function.

The consumptive use of a municipal and/or industrial complex must be part of the input data in units of acre-feet per month. This consumptive use is usually obtained from historical data concerning present and past requirements and should include modifications obtained from estimates of future population and industrial growth.

The consumptive use of irrigated area must also be part of the input data in units of acre-feet per month. An irrigated area is usually composed of several type crops with different areas for each, and the sum of these areas can represent the total area of one irrigation requirement.

Three methods are most commonly used to compute the consumptive use of an irrigated area and are stand-alone models or electronic computer programs. Two of these common methods use the Blaney-Criddle formula or a formula developed by R. L. Lowry, Jr., and A. F. Johnson.

The third method which was developed at the Engineering and Research Center of the Bureau of Reclamation in Denver, Colorado, is a stand-alone computer application titled EVPCOM (see reference 1). The consumptive use which is a theoretical value is considered as being supplied from soil moisture storage which is maintained by either irrigation applications or precipitation. The model then treats the changes in soil moisture storage as a lumped parameter on the premise that such changes are adequately reflected whenever the consumptive use requirement is met and on a monthly time frame the net effect of soil moisture storage changes are insignificant or zero.

The Penman equation is used to determine the potential transpiration rate in units of inches per day, and the crop curves of Jensen and Haise (see reference 2) are used to modify potential transpiration rate to reflect the amount of crop growth from the date of planting to the date of harvest. These modified daily rates are summed for all crops irrigated in the irrigated area for each day of each month. The summed rates for each day of the month are again summed for the month and converted to units of acre-feet per month. When precipitation is significant, it can be included in the above computation or it can be treated as a tributary inflow to the node in which the irrigated area is located.

The consumptive use for an irrigated area usually is the combination of both the nonbeneficial (miscellaneous vegetation) and the beneficial (crops) needs. The computation of the nonbeneficial use in model developed by the Bureau of Reclamation is the same as that for the beneficial use with the exception of the crop curve used which is dependent upon the type of vegetation.

Demand (Diversion Requirement)

The demands are computed in the model as functions of the consumptive use and the returnable losses. The returnable losses are obtained from historical data and are expressed as percentages of the diversion (demand). Conversely, if the consumptive use is known, the diversion or demand can be determined by dividing the consumptive use by the factor (1.0 - losses expressed as a decimal).

Return Flow

The return flow is simply the returnable losses and in the simulation it is computed as the difference between the demand and the consumptive use.

The chemistry of the return flow is determined using the premise that the consumptive use (transpiration) leaves the river basin with zero chemistry and the concentrations of the waters diverted are increased on this basis. As an example:

Let: V_1 = Volume of water diverted.

C_1 = Concentration of water diverted.

V_2 = Volume of consumptive use.

C_2 = Concentration of consumptive use = 0.

V_3 = Volume of return flow.

C_3 = Concentration of return flow.

Then: $V_3 = V_1 - V_2$

And: $C_3 = \frac{(C_1V_1 + C_2V_2)}{V_3} = \frac{C_1 \cdot V_1}{V_3}$

The array CONUSE (EQUIVALENCE KUSE) contains information designating the destination (maximum of three) and the ratio of the total return allocated to each destination.

Shortage Index

The shortage index is a function of the demand (diversion), and whenever a demand cannot be supplied within the limits of the shortage index an error message will be printed and the simulation will be terminated.

Summary

This subroutine has been designed to allow for maximum flexibility in modification for variable demand growth without resorting to a large increase in the data set. Also, if the demands for each month do not change from year to year, the demand and consumptive use cards are necessary for the first year only.

The use of the three destinations for return flow has proven to be a valuable tool in obtaining a hydraulic balance between nodes, and as a tool it can be used to improve the chemistry comparisons at the end of each node.

It has been found that a check point or response point located as far downstream in a node as possible is essential in obtaining valid results with the use of the exchange mechanism between surface and subsurface facilities. In fact, once a consistent criteria for the hydraulic balance has been established, the chemistry or salinity comparisons (observed versus predicted) will converge within reasonable limits.

The flow charts for this subroutine are shown on Figures 27 and 28. The description of variable names or data arrays is given in Table 7.

SUBROUTINE RFCOMP

REFERENCES

1. Huntley, C. W., "Computation of Consumptive Use," EVPCOM, Bureau of Reclamation Internal Document, June 1974.

2. Jensen, M. E., Wright, J. L., and Pratt, B. J., "Estimating Soil Moisture Depletion from Climate, Crops and Soil Data," Sprinkler Irrigation, 3rd Edition, 1969, Sprinkler Irrigation Association, Washington, D.C., Chapter 5, "Plant and Irrigation Water Requirements."

FLOW CHART FOR SUBROUTINE RFCOMP

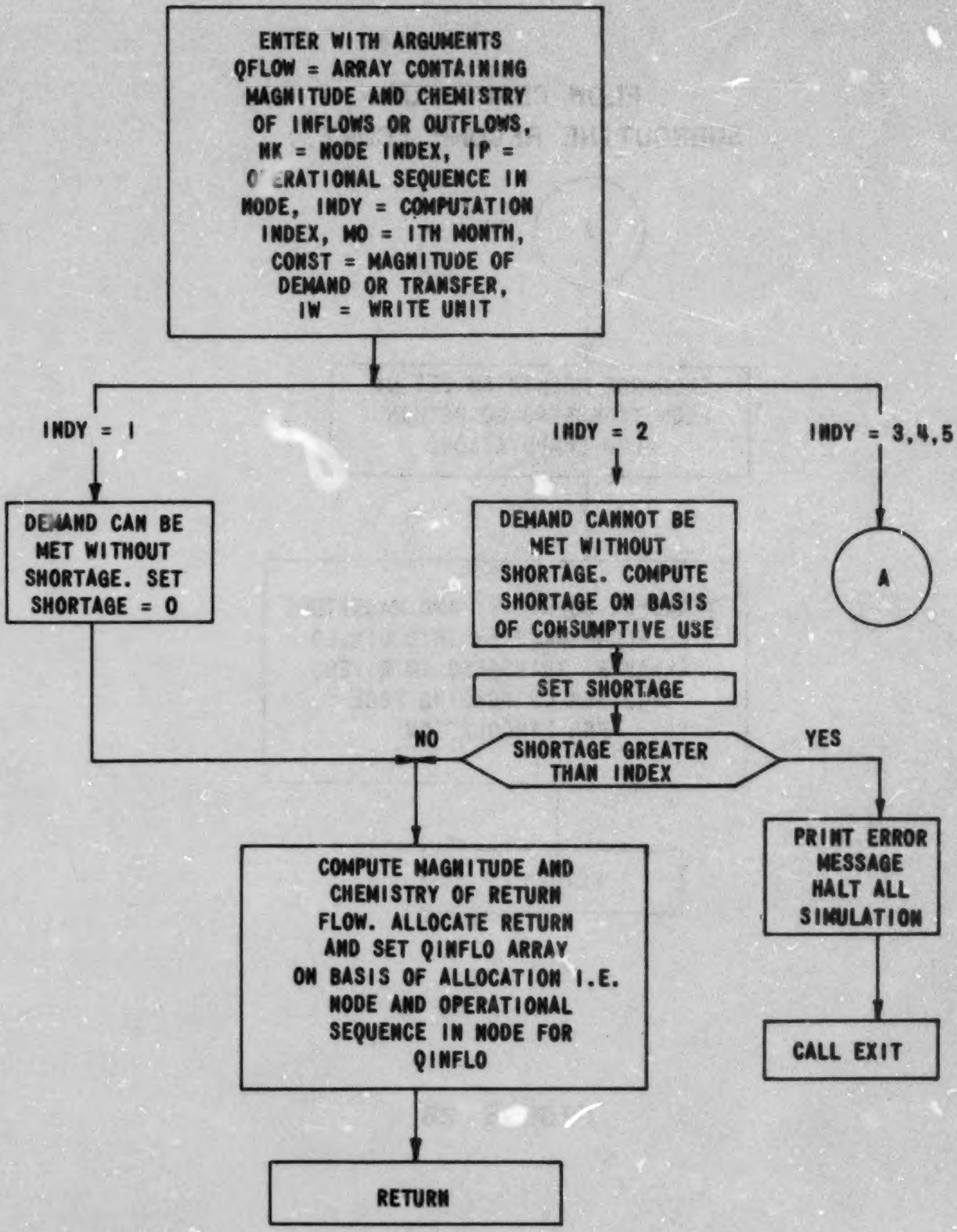

ENTER WITH ARGUMENTS QFLOW = ARRAY CONTAINING MAGNITUDE AND CHEMISTRY OF INFLOWS OR OUTFLOWS, NK = NODE INDEX, IP = OPERATIONAL SEQUENCE IN NODE, INDY = COMPUTATION INDEX, MO = ITH MONTH, CONST = MAGNITUDE OF DEMAND OR TRANSFER, IW = WRITE UNIT
INDY = 1
INDY = 2
INDY = 3,4,5
DEMAND CAN BE MET WITHOUT SHORTAGE. SET SHORTAGE = 0
DEMAND CANNOT BE MET WITHOUT SHORTAGE. COMPUTE SHORTAGE ON BASIS OF CONSUMPTIVE USE
A
SET SHORTAGE
NO
SHORTAGE GREATER THAN INDEX
YES
COMPUTE MAGNITUDE AND CHEMISTRY OF RETURN FLOW. ALLOCATE RETURN AND SET QINFLO ARRAY ON BASIS OF ALLOCATION I.E. NODE AND OPERATIONAL SEQUENCE IN NODE FOR QINFLO
PRINT ERROR MESSAGE HALT ALL SIMULATION
CALL EXIT
RETURN

FIGURE 27

FLOW CHART FOR SUBROUTINE RFCOMP (CONT.)

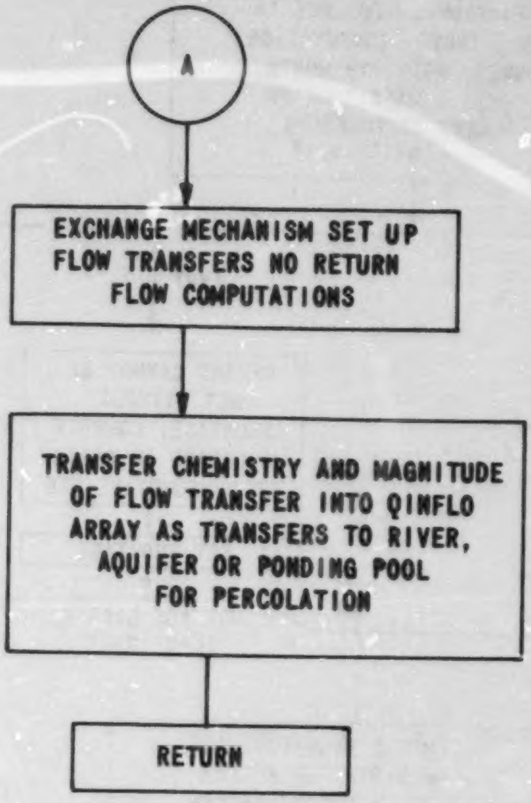

A
EXCHANGE MECHANISM SET UP FLOW TRANSFERS NO RETURN FLOW COMPUTATIONS
TRANSFER CHEMISTRY AND MAGNITUDE OF FLOW TRANSFER INTO QINFLO ARRAY AS TRANSFERS TO RIVER, AQUIFER OR PONDING POOL FOR PERCOLATION
RETURN

FIGURE 28

Table 7

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE RFCOMP

Variable name	C*	Description	Remarks or units
CONST		Constant used to store magnitude of demand	Acre-feet
CONUSE	C	Consumptive use array storing various pertinent parameters	See previous definition of data array CONUSE
DEMAND	C	Array used to store magnitude of demands on monthly basis in acre-feet	See previous definition of data array DEMAND
INDY		Computation index	
IP		Operational sequence in node	
IW		Write unit designation	
JK		Node sequence in setting QINFLO array	
KA		Loop index	
KDEMNM	C	Alpha description of demand or diversion	
KDES		Destination index of return and transfer flows (3 character alpha)	
KNODE		Node number of return flow allocation and flow transfer	
K		Loop index	
KSEQ		Operational sequence in node of return flow or flow transfer	

Table 7 - Continued

Variable name	C*	Description	Remarks or units
KUSE	C	Integer equivalence of consumptive use array	Equivalence of array CONUSE
MO		I_{th} month in simulation	
NFIND		Entry to subroutine NFIND	See subroutine NFIND
NK		Node index	
PER		Distribution ratio for return flow allocation	
QFLOW		Array containing magnitude and chemistry of inflow or outflow	See data array QFLOW
QINFLO		Array containing parameters of tributary inflow	See previously defined data array QINFLO
RATIO		Decimal equivalent of conveyance and farm losses or conveyance and municipal or industrial losses	
RFLOW		Return or excess flow from a diversion either irrigation or municipal and/or industrial demand	See data array RFLOW
SHORT		Actual shortage in supplying ideal demand (diversion) in percent of consumptive use requirement or ideal demand	
TEMCU		Computational aid in computing consumptive use shortage	
VOLA		Computational aid for volume in computing chemistry of return flow	Acre-feet
VOLB		Same purpose as VOLA	Acre-feet

Table 7 - Continued

DATA ARRAY QFLOW (10)

QFLOW (1) = Magnitude of demand or transfer in acre-feet

QFLOW (2) = Concentration of calcium in parts per million

QFLOW (3) = Concentration of magnesium

QFLOW (4) = Concentration of sodium

QFLOW (5) = Concentration of chloride

QFLOW (6) = Concentration of sulfate

QFLOW (7) = Concentration of bicarbonate

QFLOW (8) = Concentration of carbonate

QFLOW (9) = Concentration of nitrate

QFLOW (10) = Concentration of total salts (TDS)

DATA ARRAY RFLOW (10)

RFLOW (1) = Magnitude of return flow in acre-feet

RFLOW (2-10) = Same as QFLOW (2-10)

SUBROUTINE CHEMGR

This subroutine simulates the mixing of waters of different chemical composition as the waters are intercepted at a common point. The subroutine has seven entry points to facilitate the mixing calls from several sources.

The argument list consists of an array containing the magnitude and chemistry of both the incoming and outgoing waters, a constant, the node index, and the operational sequence of the node.

All of the mixing equations contained in this subroutine are linear as the following example indicates.

Let: V_1 = Volume of water to be mixed from the first source.

C_{1j} = Concentration in ppm of the j_{th} constituent from the first water source.

V_2 = Volume of water to be mixed from the second source.

C_{2j} = Concentration in ppm of the j_{th} constituent from the second water source.

V_3 = Combined volume of first and second sources.

C_{3j} = Combined concentration in parts per million of the j_{th} constituent of the first and second sources.

$$C_{3j} = \frac{(V_1C_{1j} + V_2C_{2j})}{V_3}$$

It is a simple task to modify any of the mixing equations to include nonlinear relationships if information and data justify such a representation.

A flow chart of this subroutine is shown on Figures 29 and 30. The variable names or arrays are shown in Table 8.

Subroutine CHEMGR is a multiple entry device with six entry points. These entry points are designated on Figures 29 and 30 with an appropriate description as to function of each entry point.

FLOW CHART FOR
SUBROUTINE CHEMGR

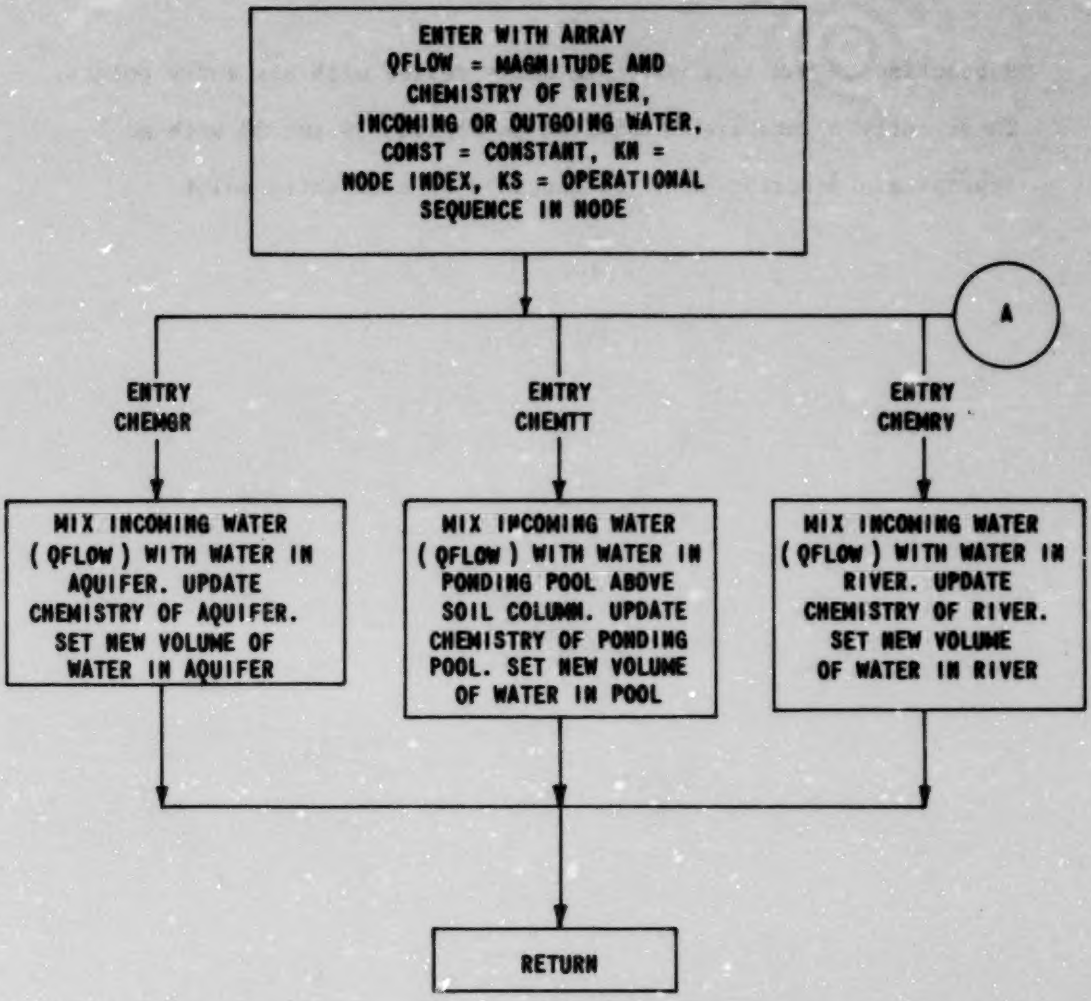

ENTER WITH ARRAY QFLOW = MAGNITUDE AND CHEMISTRY OF RIVER, INCOMING OR OUTGOING WATER, CONST = CONSTANT, KN = NODE INDEX, KS = OPERATIONAL SEQUENCE IN NODE
A
ENTRY CHEMGR
ENTRY CHEMTT
ENTRY CHEMRV
MIX INCOMING WATER (QFLOW) WITH WATER IN AQUIFER. UPDATE CHEMISTRY OF AQUIFER. SET NEW VOLUME OF WATER IN AQUIFER
MIX INCOMING WATER (QFLOW) WITH WATER IN PONDING POOL ABOVE SOIL COLUMN. UPDATE CHEMISTRY OF PONDING POOL. SET NEW VOLUME OF WATER IN POOL
MIX INCOMING WATER (QFLOW) WITH WATER IN RIVER. UPDATE CHEMISTRY OF RIVER. SET NEW VOLUME OF WATER IN RIVER
RETURN

FIGURE 29

FLOW CHART FOR SUBROUTINE CHEMGR (CONT)

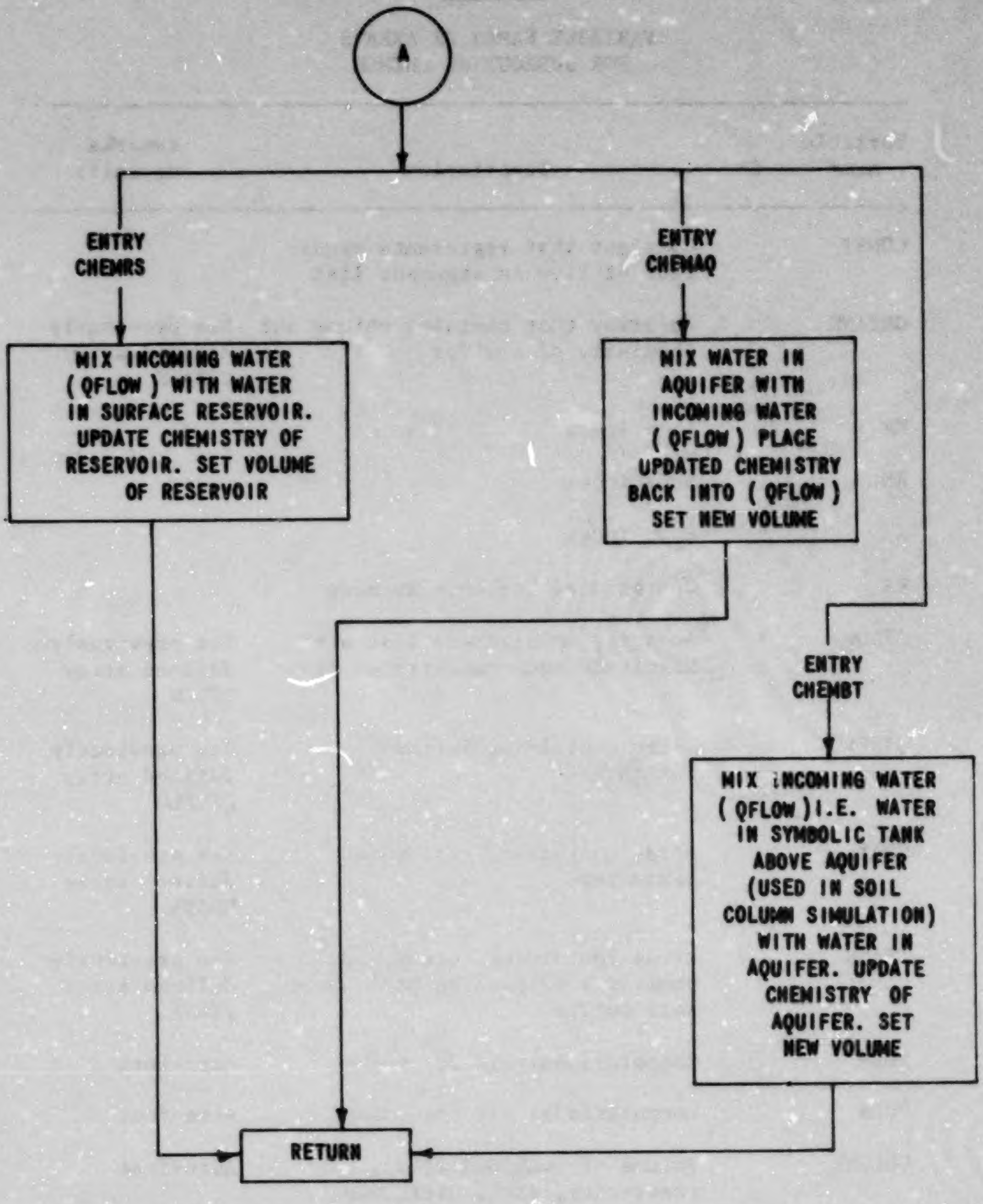

A
ENTRY CHEMRS
ENTRY CHEMAQ
MIX INCOMING WATER (QFLOW) WITH WATER IN SURFACE RESERVOIR. UPDATE CHEMISTRY OF RESERVOIR. SET VOLUME OF RESERVOIR
MIX WATER IN AQUIFER WITH INCOMING WATER (QFLOW) PLACE UPDATED CHEMISTRY BACK INTO (QFLOW) SET NEW VOLUME
ENTRY CHEMBT
MIX INCOMING WATER (QFLOW) I.E. WATER IN SYMBOLIC TANK ABOVE AQUIFER (USED IN SOIL COLUMN SIMULATION) WITH WATER IN AQUIFER. UPDATE CHEMISTRY OF AQUIFER. SET NEW VOLUME
RETURN

FIGURE 30

Table 8

VARIABLE NAMES OR ARRAYS FOR SUBROUTINE CHEMGR

Variable name	C*	Description	Remarks or units
CONST		Constant that represents magnitude of flow in argument list	
GRTANK		An array that contains volume and chemistry of aquifer	See previously defined array GRTANK
KA		Loop index	
KN		Node index	
K		Loop index	
KS		Operational sequence in node	
QFLOW		An array in argument list with magnitude and chemistry of flow	See previously defined array QFLOW
QINFLO		Array containing inflow parameters	See previously defined array QINFLO
RDATA		Array containing reservoir parameters	See previously defined array RDATA
TTANK		Array containing volume and chemistry of ponding pool above soil column	See previously defined array TTANK
VOLA		Computational aid for volume	Acre-feet
VOLB		Computational aid for volume	Acre-feet
VOLUME		Volume of combined flows, reservoirs, etc., after mix	Acre-feet

SUBROUTINE CONVER

This subroutine is used to convert units of concentration from milliequivalents per liter to parts per million. Parts per million are the units used throughout the simulation with the exception of that portion simulating waters percolating vertically through a soil column.

The argument list contains an array of the constituents to be converted and an index signifying if the incoming units of concentration are in parts per million or in milliequivalents per liter. When this index is equal to one, the units are in milliequivalents per liter.

The subroutine checks the balance of anions and cations with the use of the concentrations of the eight constituents in units of equivalents when such concentrations are given as part of the input data set. The difference between the sum of cations and the sum of anions (if any) is added to the concentrations of the calcium or the sulfate constituent dependent upon which of the sums is larger. It is obvious that not all of the constituents in a sample can be represented as eight constituents; therefore, this check is not an explicit representation of a mass balance. The use of this premise does not extend a significant error and does provide continuity for subsequent requirements for a mass balance. When the concentrations of constituents are not a part of the input data set, the balance of ions is bypassed as well as the computation of total salts (TDS).

The total salts are computed with the use of the concentrations of the eight constituents when such data is part of the data set. This computation is performed in units of parts per million, and one-half of the concentration of the bicarbonate constituent is used in the computation.

The variable names or arrays are shown in Table 9.

Table 9

VARIABLE NAMES OR ARRAYS
FOR SUBROUTINE CONVER

Variable name	C*	Description	Remarks or units
DIFF		Difference between sum of cations and anions	ppm
EQVWT		Equivalent weight array for constituents	See data array EQVWT
SUMA		Sum of anions	ppm
SUMC		Sum of cations	ppm
TDS		Total salts	ppm
TEMP		Incoming array of constituents	See data array TEMP

DATA ARRAY TEMP (15)

TEMP (2) = Concentration of calcium

TEMP (3) = Concentration of magnesium

TEMP (4) = Concentration of sodium

TEMP (5) = Concentration of chloride

TEMP (6) = Concentration of sulfate

TEMP (7) = Concentration of bicarbonate

TEMP (8) = Concentration of carbonate

TEMP (9) = Concentration of total salts

TEMP (10) = Total salts

DATA ARRAY EQVWT (8)

EQVWT (1) = Equivalent weight of calcium = 20.04

Table 9 - Continued

DATA ARRAY EQVWT (8) - Continued

EQVWT (2) = Equivalent weight of magnesium = 12.16

EQVWT (3) = Equivalent weight of sodium = 23.0

EQVWT (4) = Equivalent weight of chloride = 35.46

EQVWT (5) = Equivalent weight of sulfate = 48.03

EQVWT (6) = Equivalent weight of bicarbonate =30.0

EQVWT (7) = Equivalent weight of carbonate = 61.01

EQVWT (8) = Equivalent weight of nitrate = 62.008

SUBROUTINE VERNAL

This subroutine is used for the simulation of the operational criteria for the Vernal Project Study. A subroutine such as this will have to be designed for each river basin simulated using this model.

The operational criteria differ considerably from one river basin to another, and any attempt to generalize this portion of the model would be futile.

It is believed that a near maximum use of all the model features would require several subroutines to include all the needs of a complex operational criteria. In such a case it is recommended that a monitor subroutine with one or two calls from the main or executive program be utilized to maintain the flexibility of the model.

This subroutine as written contains the very simple operational criteria for the three node Vernal Project. The flow chart of the subroutine is shown on Figure 31.

FLOW CHART FOR SUBROUTINE VERNAL

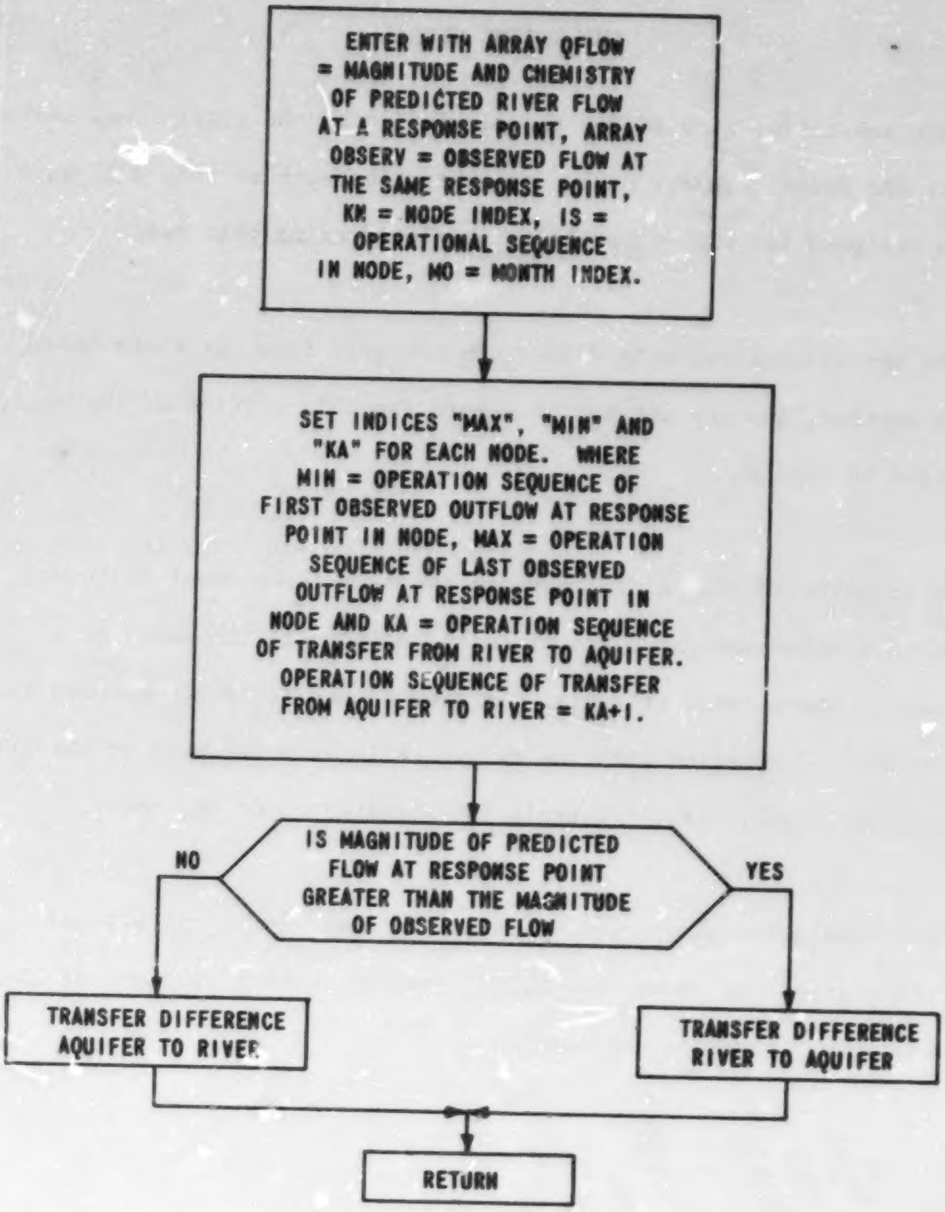

ENTER WITH ARRAY QFLOW = MAGNITUDE AND CHEMISTRY OF PREDICTED RIVER FLOW AT A RESPONSE POINT, ARRAY OBSERV = OBSERVED FLOW AT THE SAME RESPONSE POINT, KN = NODE INDEX, IS = OPERATIONAL SEQUENCE IN NODE, MO = MONTH INDEX.
SET INDICES "MAX", "MIN" AND "KA" FOR EACH NODE. WHERE MIN = OPERATION SEQUENCE OF FIRST OBSERVED OUTFLOW AT RESPONSE POINT IN NODE, MAX = OPERATION SEQUENCE OF LAST OBSERVED OUTFLOW AT RESPONSE POINT IN NODE AND KA = OPERATION SEQUENCE OF TRANSFER FROM RIVER TO AQUIFER. OPERATION SEQUENCE OF TRANSFER FROM AQUIFER TO RIVER = KA+1.
IS MAGNITUDE OF PREDICTED FLOW AT RESPONSE POINT GREATER THAN THE MAGNITUDE OF OBSERVED FLOW
NO
YES
TRANSFER DIFFERENCE AQUIFER TO RIVER
TRANSFER DIFFERENCE RIVER TO AQUIFER
RETURN

FIGURE 31

FUNCTION ROOTWO

This function was found very useful in the simulation because of the several requirements throughout the model for the solution of a root for quadratic equations. The roots of these quadratic equations by definition must be real and unequal because all the coefficients of the quadratic are real. A criteria that no imaginary roots can exist is signaled by a write statement included in the function. The solution of the quadratic equation for a single root is as follows:

$$x = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

where: $ax^2 + bx + c = o$ and $a \neq o$

The argument list for this subroutine consists of the node index, operational sequence in the node, an array of the coefficients in decreasing powers of "x", a six alpha character indentifier designating the origin of the call and the write unit designation. The variable names and arrays are shown in Table 10.

Table 10

VARIABLE NAMES OR ARRAYS FOR FUNCTION ROOTWO

Variable name	C*	Description	Remarks or units
CA		An array containing the coefficients of the quadratic equation	See data array CA
IW		Write unit designation	
KNODE		Node index	
KSEG		Operational sequence in node	
MOLE		Six character alpha designation of calling routine	
RAD		Radical term in the solution of a quadratic equation	

DATA ARRAY CA(10)

CA(1) = "a" coefficient

CA(2) = "b" coefficient

CA(3) = "c" coefficient

Quadratic equation = $ax^2 + bx + c$

FUNCTION ROOT

This subroutine is used to solve for a real root of an nth degree polynomial given that such a root lies between two limits and assuming that only one real root exists within these limits.

The technique used is a combination of the Newton or Newton-Raphson method where the first derivative is approximated (Regula falsi) and an algorithm for the solution of a polynomial (Function FOFX). The subroutine was designed primarily for the solution of the more complex functions; consequently, the necessity for approximating the first derivative. In the model this subroutine is used to find roots of those polynomials higher than second degree.

The argument list contains a constant, the upper limit of the root, the lower limit of the root, a five alpha character designation for the validity of the root, an array containing the coefficients of the polynomial and a test constant for convergence.

A brief description of the procedure is:

given a polynomial, i.e.

$$f(X) = a_1X^n + a_2X^{n-1} + \dots + a_nX + a_{n+1}$$

where n = degree of polynomial, $n > 2$

find a root X_r, where: $X_{min} \leq X_r \leq X_{max}$

The Newton or Newton-Raphson method is formulated as follows:

$$X_{n+1} = X_n - \frac{f(X_n)}{f'(X_n)}$$

Let the approximation (Regula falsi) of $f'(X_n)$ be:

$$f'(X_n) \sim \frac{f(X_n) - f(X_{n-1})}{X_n - X_{n-1}}$$

Upon substitution then:

$$X_{n+1} = X_n - \frac{f(X_n)}{\dfrac{f(X_n) - f(X_{n-1})}{X_n - X_{n-1}}}$$

or:

$$X_{n+1} = X_n - \frac{(X_n - X_{n-1})f(X_n)}{f(X_n) - f(X_{n-1})}$$

Let the first seed (guess) be:

$$X_{n-1} = X_{min}$$

$$X_n = X_{n-1} + 0.1\, X_{min}$$

Begin iterative procedure with maximum of 20 iterations or until $[X_{n+1} - X_n] \leq \epsilon$.

This function calls the function FOFX for the evaluation of the polynomial using the algorithm described in function FOFX.

When the root (X_r) is within the limits of X_{min} and X_{max} the alpha designator will be set as TRUE, when the root exceeds the limits the alpha designator will be set as FALSE, and when the number of iterations exceeds 20 the alpha indicator will be set as NONE.

The method used to evaluate the polynomial requires the coefficients of the polynomial to be passed in increasing powers of the independent variable, i.e.:

$$f(x) = a_0 + a_1 X + a_2 X^2 + \ldots + a_n X^n$$

where n = degree of polynomial.

The indexing format of the coefficient array in the computer application prohibits the use of zero; therefore the function will actually be represented as follows:

$$f(x) = a_1 + a_2 X + a_3 X^2 + \ldots + a_{n+1} X^n$$

If - $f(x) = K = a_1 + a_2 X + a_3 X^2 + \ldots + a_{n+1} X^n$

then: $f(x) = 0 = a_1 - K + a_2 X + a_3 X^2 + \ldots + a_{n+1} X^n$

The flow chart for this function is shown on Figure 32. The variable names and arrays are shown in Table 11.

FLOW CHART FOR FUNCTION ROOT

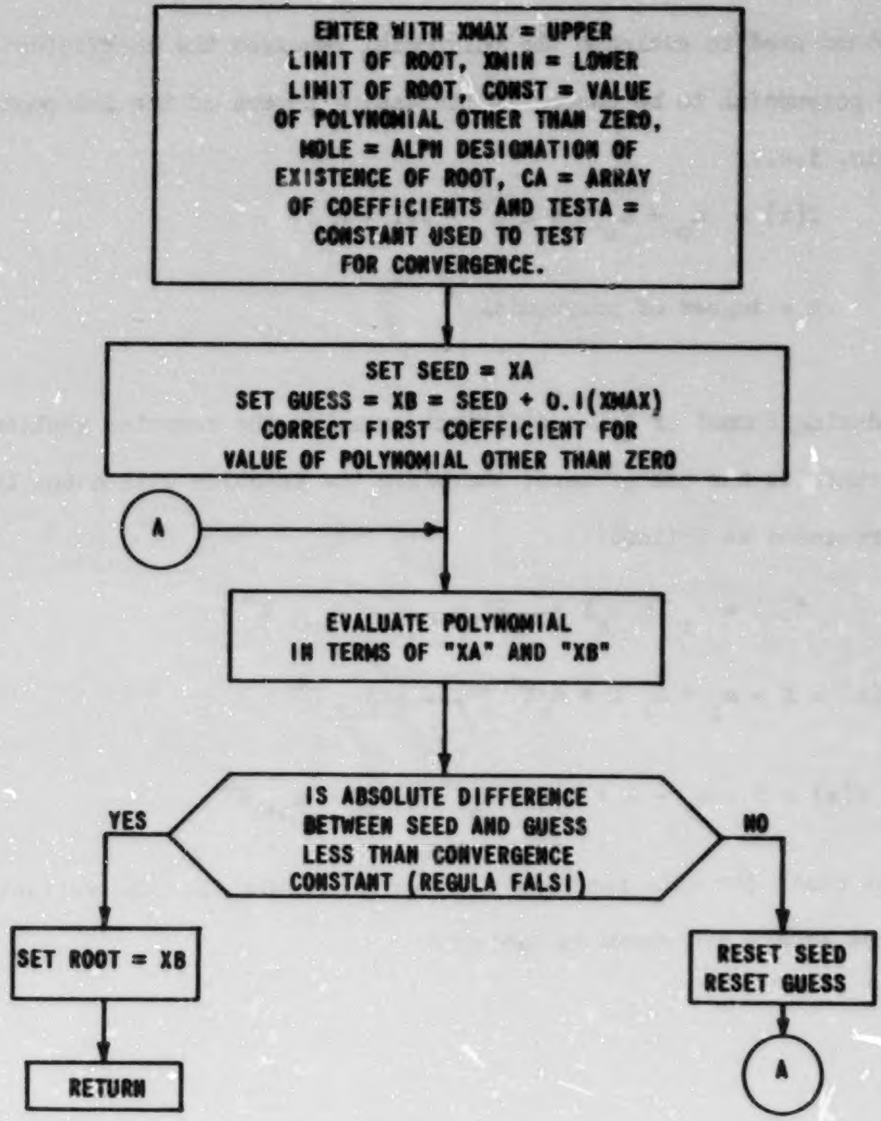

ENTER WITH XMAX = UPPER LIMIT OF ROOT, XMIN = LOWER LIMIT OF ROOT, CONST = VALUE OF POLYNOMIAL OTHER THAN ZERO, MOLE = ALPH DESIGNATION OF EXISTENCE OF ROOT, CA = ARRAY OF COEFFICIENTS AND TESTA = CONSTANT USED TO TEST FOR CONVERGENCE.
SET SEED = XA
SET GUESS = XB = SEED + 0.1(XMAX)
CORRECT FIRST COEFFICIENT FOR VALUE OF POLYNOMIAL OTHER THAN ZERO
A
EVALUATE POLYNOMIAL IN TERMS OF "XA" AND "XB"
IS ABSOLUTE DIFFERENCE BETWEEN SEED AND GUESS LESS THAN CONVERGENCE CONSTANT (REGULA FALSI)
YES
NO
SET ROOT = XB
RETURN
RESET SEED
RESET GUESS
A

FIGURE 32

Table 11

VARIABLE NAMES OR DATA ARRAYS FOR FUNCTION ROOT

Variable name	C*	Description	Remarks or units
CA		Array containing coefficients of polynomial	See data array CA
CONST		Used when $f(x) = K =$ CONST	
DXDP		Variable name for $f(X_n) - f(X_{n-1})$	
DX		Variable name for $X_n - X_{n-1}$	
EPSLON		Variable name for $[X_{n+1} - X_n]$	
FOFX		Entry to function FOFX	See Subroutine FOFX
FXA		Variable name for $f(X_{n-1})$	
FXB		Variable name for $f(X_n)$	
IW		Write unit designation	
K		Loop index	
MOLE		Five-character alpha designator of root	
NK		Iteration counter	
ROOT		Variable name for X_r	
TESTA		Convergence term for iterative scheme	
XA		Variable name for X_{n-1}	
XB		Variable name for X_n	
XC		Variable name for X_{n+1}	

Table 11 - Continued

VARIABLE NAMES OR DATA ARRAYS
FOR FUNCTION ROOT

Variable name	C*	Description	Remarks or units
XMAX		Variable name for upper limit of root	
XMIN		Variable name for lower limit of root	

DATA ARRAY CA (10)

CA (1) = Coefficient for X^n

CA (2) = Coefficient for X^{n-1}

CA(10) = Coefficient for X^0

The number of coefficients will always be one greater than the degree of the polynomial; however, the coefficient for X^n must always be stored in CA(1) and the index of the array CA will increase as the power of "X" decreases in the polynomial.

FUNCTION FOFX

This function was designed to evaluate any polynomial of degree n from n = 1 to n = 9; however, in the model it is set to evaluate polynomials from n = 1 to n = 4.

The argument list consists of the array containing the coefficients, the value of "X" in the polynomial to be evaluated and an indicator used to clear the coefficient array after the evaluation of the polynomial.

The function uses the following algorithm in the evaluation of the polynomial:

given - $'f(x) = a_0 + a_1 X + a_2 X^2 + \dots + a_n X^n$

which can be rewritten as follows:

$$f(x) = a_0 + X \left[a_1 + X [a_2 + X (a_3 + \dots)] \right]$$

Thus, $(a_n X + a_{n-1})$ can be generated and then multiplied by X and added to a_{n-2}. The process is repeated until the final addition of a_0 is made.

It is obvious that the above algorithm will be valid when the indexing of the coefficients begins with one rather than zero.

SUBROUTINE SOILCO

This subroutine monitors several other subroutines that are used to simulate the chemical exchange (inorganic) between the soil and water as water percolates vertically through a soil column. This subroutine is called from the main or executive program at the completion of the node balance at the end of each time frame.

The argument list consists of the node index, the write indicator, the read indicator, and the number of segments in the soil column.

An early version of simulating the exchanges that take place in the chemistry of waters percolating through a soil column was based upon a model developed by Dr. Gordon R. Dutt, a staff member of the University of Arizona. Subsequently, a more elaborate model was developed at the University of Arizona by Drs. Gordon R. Dutt, Marvin J. Shaffer, and William J. Moore for the predictions of the ion exchanges between the applied waters and the soil complex. This particular model is described in the University of Arizona Technical Bulletin 196, dated October 1972 and titled "Computer Simulation Model of Dynamic Bio-Physicochemical Processes in Soils."

A study was made of the Technical Bulletin 196 and the early version of the soil column simulation was modified using the more recent techniques as contained in the aforementioned bulletin. In this simulation model the interest is only in the prediction of changes in salinity. Therefore, the soil column simulation predicts only the changes in concentration of calcium, magnesium, sodium, sulfate, carbonate, bicarbonate, and the concentrations of undissociated calcium and magnesium sulfates. The soil column simulation does not involve chemical reactions with the nitrate and chloride constituents. Neglecting the chemical reactions of these two constituents does not impair the ionic balance.

Most laboratory analyses of the soil extract report concentrations of the constituents in solution in units of milliequivalents per liter.

An equivalent weight is defined as the formula weight of a constituent divided by its valence; i.e., $SO_4^=$ has a formula weight of 96.06 grams and has a valence of two; hence, the equivalent weight of $SO_4^=$ (sulfate) is 96.06/2 = 48.03 grams.

The computational mode of the soil column simulation requires the concentrations of the constituents be expressed in units of mols (moles) per liter. A mol is defined as the formula weight of a constituent per liter of solution. It follows from the above definitions that valence is equal to equivalents per mol. The dimensional characteristics of the conversion from milliequivalents per liter to mols per liter are as follows:

Let: milliequivalents = meq = equivalents (10^{-3})

and: (equivalents/liter) (mols/equivalent) = mols/liter

then: (meq/liter/valence) (10^{-3}) = mols/liter

In the solid phase (soil) concentrations are reported in milliequivalents per 100 grams of soil.

The concentrations of the solid phase (soil) in the computational mode are in units of mols per gram. The dimensional characteristics of this conversion are as follows:

Let: milliequivalents/100 grams = meq/grams(10^{2})

then: $$\text{meq/grams}(10^{2}) = \frac{\text{equivalents}}{\text{grams}} (10^{-5})$$

and: $$(\text{equivalents/grams})\ (10^{-5})\ \frac{1}{\text{equivalents/mol}} = \frac{\text{mols}}{\text{gram}}$$

then: (meq/100 grams) / (valence(10^{5})) = mols/gram

A very important parameter in the simulation of applied waters percolating through a soil column is the moisture content of the soil. It is obvious that this parameter changes for each small time increment and is dependent upon the variations of applied waters for irrigation, municipal or industrial requirements, precipitation, and the soil composition. A study of the variations of applied water and the homogeneity of the soil in the area to be simulated must be made to determine a reasonable value for the moisture content on a monthly basis. The difficulty in the determination of moisture content (field conditions) should not be under emphasized, or for that matter the selection of a representative soil composition for a large area.

In some river basins the soil column simulation is not required or has little impact upon the prediction of changes in salinity (chemistry), and in such circumstances the soil column simulation can be eliminated by simply not including any soil data in the overall data set.

The soil extract in a laboratory analysis is commonly made by adding one gram of water to one gram of oven-dried soil to produce a one to one soil-water ratio. The definition of a soil extract represents the solution separated from a soil suspension, and also by definition moisture content is the ratio of the weight of water to the weight of soil. The percentage moisture approximates the (weight of water/weight of soil) (100).

Field capacity is defined as the moisture content in the soil 2 or 3 days after a thorough wetting of the soil profile by precipitation or irrigation.

It might be well to mention that most results of the analysis of the chemical composition of waters are reported in units of parts per million which is a weight to weight unit. To convert parts per million to milliequivalents per liter, simply divide parts per million by the equivalent weight of the constituent; also, it can be easily shown that equivalents per million and milliequivalents per liter are numerically equal.

The volume of water per soil segment which is part of the input data is used to compute the moisture content. The bulk density, which is defined as the ratio of the weight of oven-dried soil to the field volume of the soil, and the length of the soil segment in centimeters are also used to compute moisture content. The computation is as follows:

Moisture content = (Weight of water (grams)/segment)
/ (Bulk density · length of segment
unit area of segment)

Dimensionally:

$$\text{Moisture content} = (\text{grams } H_2O/\text{segment})/(\text{grams of soil}/cm^3)\ (cm^2)\ (^{cm}/\text{segment}) = \frac{\text{grams } H_2O}{\text{grams soil}}$$

The movement of the percolating waters through the soil column is on the basis of a "piston effect"; i.e., the solution contained in one segment is moved to the next lower segment and then equilibrated with the soil characteristics of lower segment. A diagram of this logic is shown on Figure 33.

A diagram with the symbolic names used in the soil column simulation is shown on Figure 34. The flow chart is shown on Figures 35 through 38, and the table of variable names and arrays is shown in Table 12.

LOGIC OF PISTON EFFECT OF SOLUTION MOVING VERTICALLY THROUGH A SOIL COLUMN (THREE SEGMENTS)

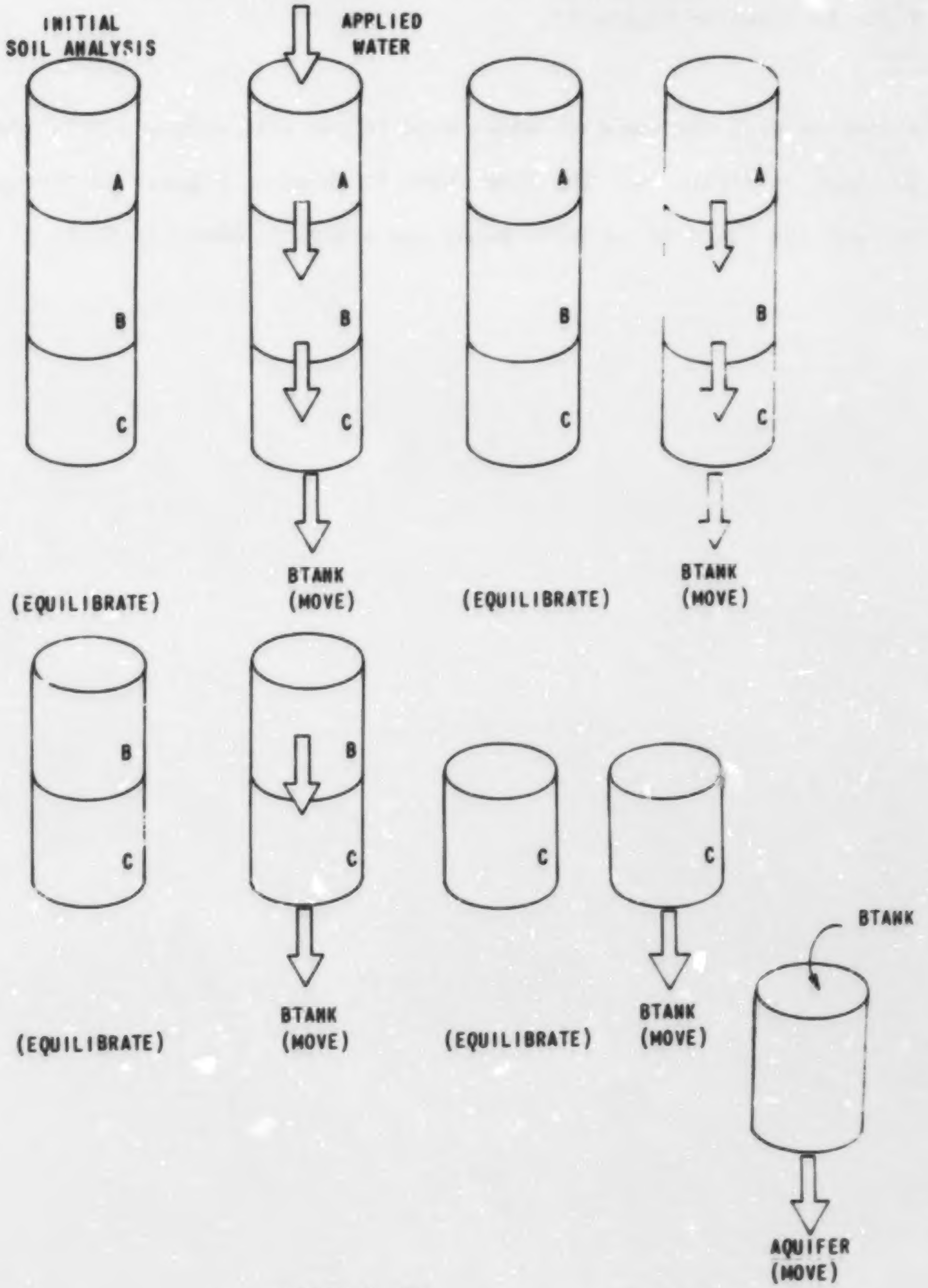

INITIAL
SOIL ANALYSIS
APPLIED
WATER
A
B
C
(EQUILIBRATE)
BTANK
(MOVE)
(EQUILIBRATE)
BTANK
(MOVE)
(EQUILIBRATE)
BTANK
(MOVE)
(EQUILIBRATE)
BTANK
(MOVE)
BTANK
AQUIFER
(MOVE)

FIGURE 33

SYMBOLIC NAMES USED IN SIMULATION OF SOIL COLUMN

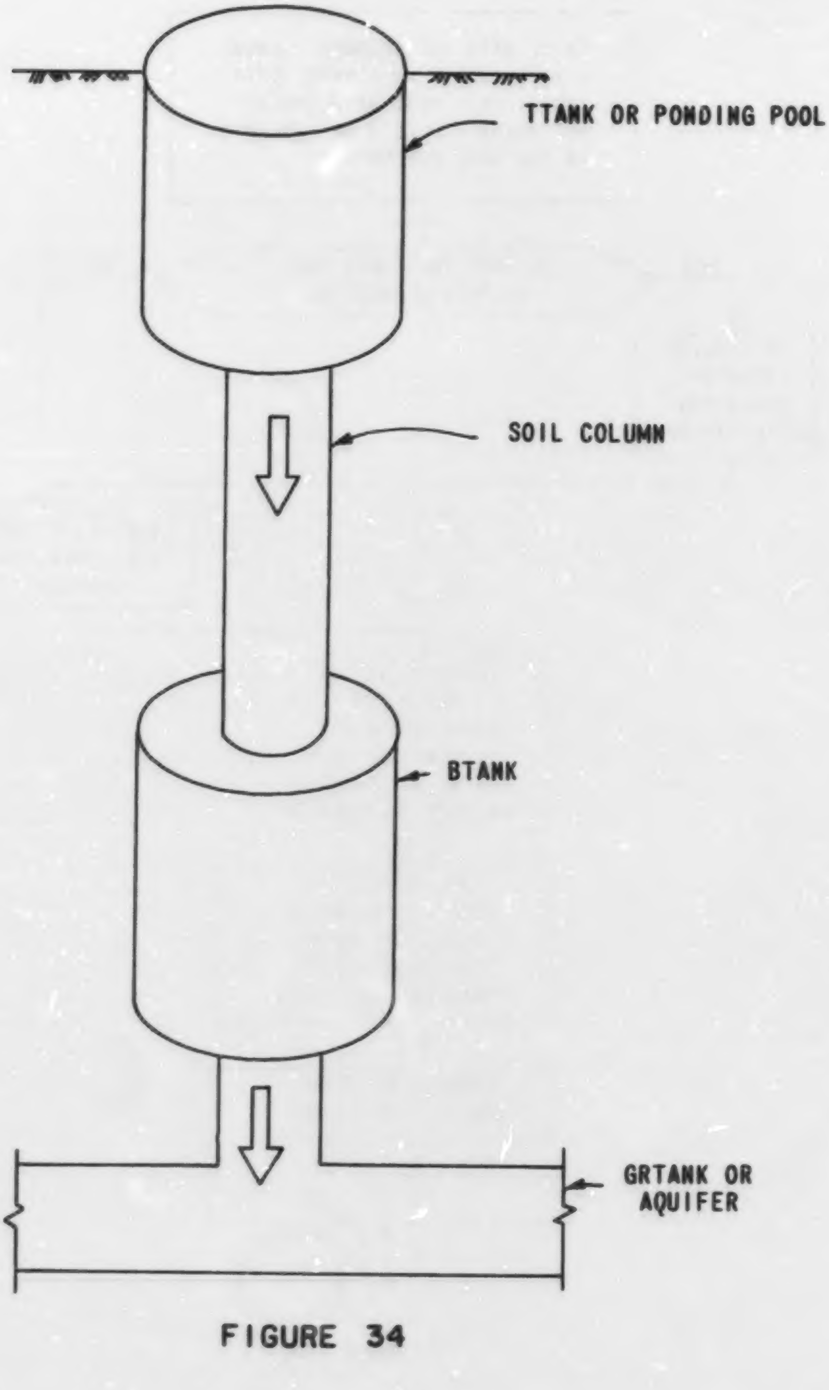

TTANK OR PONDING POOL
SOIL COLUMN
BTANK
GRTANK OR AQUIFER

FIGURE 34

FLOW CHART FOR SUBROUTINE SOILCO

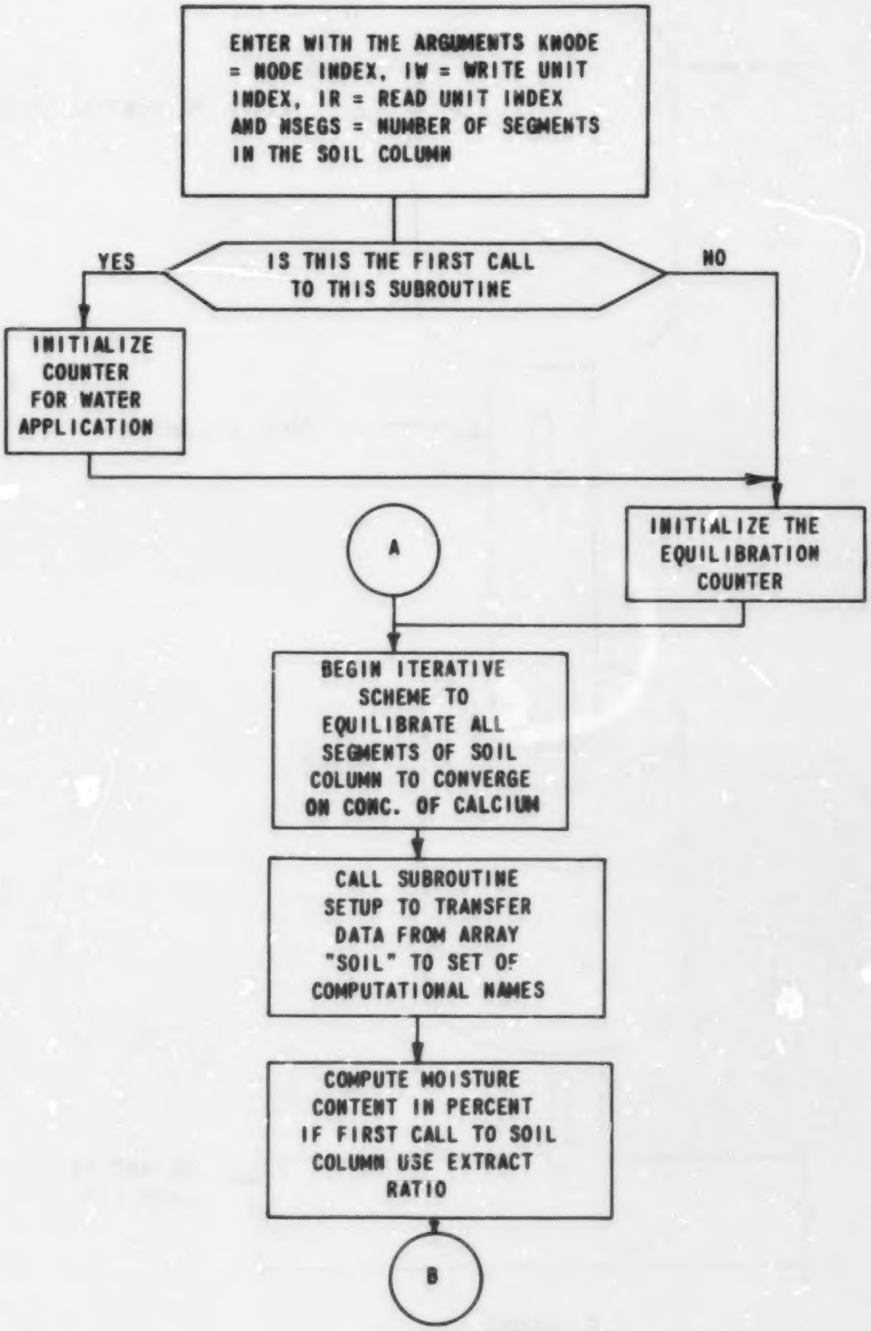

ENTER WITH THE ARGUMENTS KNODE = NODE INDEX, IW = WRITE UNIT INDEX, IR = READ UNIT INDEX AND NSEGS = NUMBER OF SEGMENTS IN THE SOIL COLUMN
IS THIS THE FIRST CALL TO THIS SUBROUTINE
YES
NO
INITIALIZE COUNTER FOR WATER APPLICATION
INITIALIZE THE EQUILIBRATION COUNTER
A
BEGIN ITERATIVE SCHEME TO EQUILIBRATE ALL SEGMENTS OF SOIL COLUMN TO CONVERGE ON CONC. OF CALCIUM
CALL SUBROUTINE SETUP TO TRANSFER DATA FROM ARRAY "SOIL" TO SET OF COMPUTATIONAL NAMES
COMPUTE MOISTURE CONTENT IN PERCENT IF FIRST CALL TO SOIL COLUMN USE EXTRACT RATIO
B

FIGURE 36

FLOW CHART FOR
SUBROUTINE SOILCO (cont.)

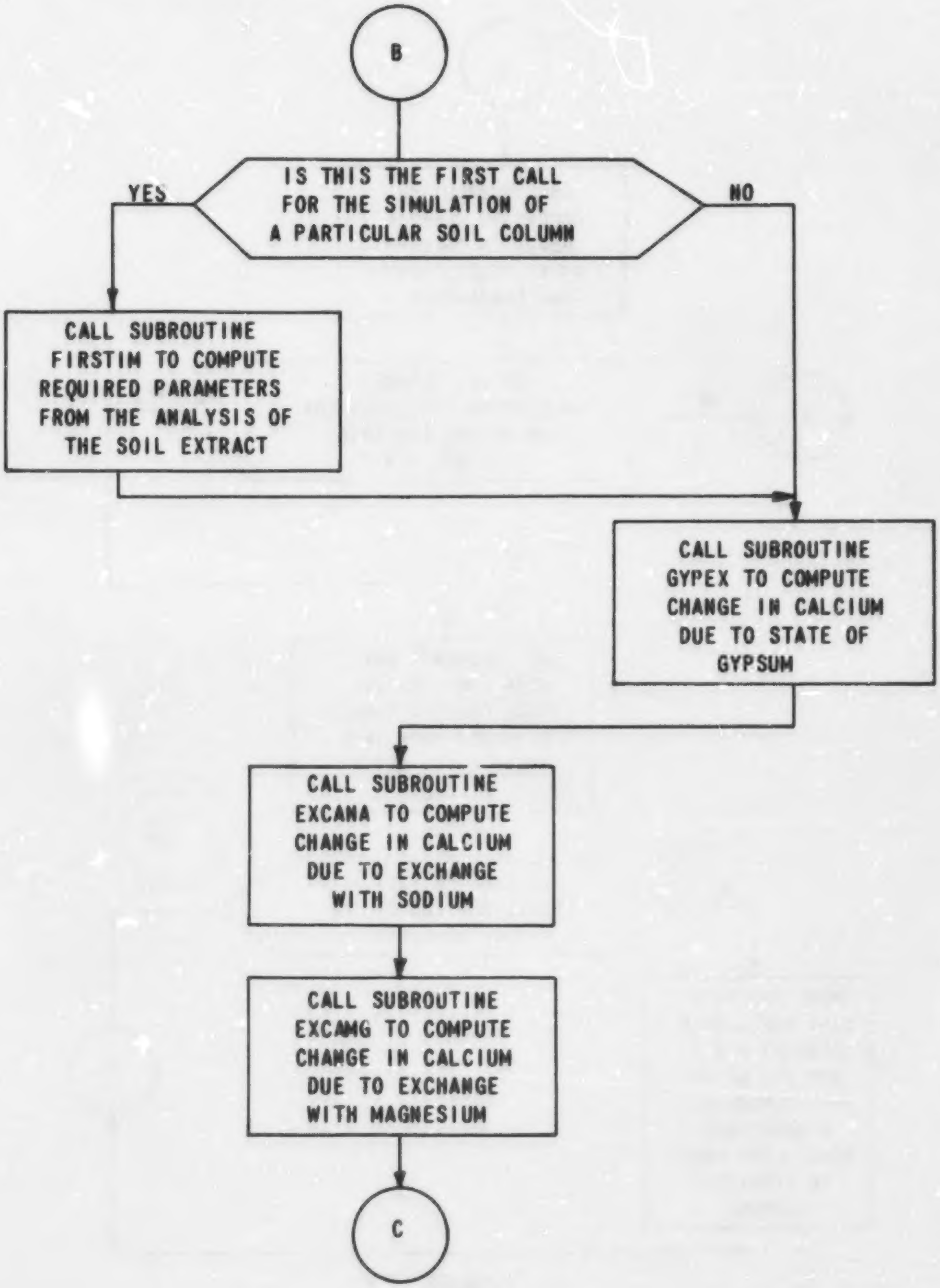

B
IS THIS THE FIRST CALL FOR THE SIMULATION OF A PARTICULAR SOIL COLUMN
YES
NO
CALL SUBROUTINE FIRSTIM TO COMPUTE REQUIRED PARAMETERS FROM THE ANALYSIS OF THE SOIL EXTRACT
CALL SUBROUTINE GYPEX TO COMPUTE CHANGE IN CALCIUM DUE TO STATE OF GYPSUM
CALL SUBROUTINE EXCANA TO COMPUTE CHANGE IN CALCIUM DUE TO EXCHANGE WITH SODIUM
CALL SUBROUTINE EXCAMG TO COMPUTE CHANGE IN CALCIUM DUE TO EXCHANGE WITH MAGNESIUM
C

FIGURE 35

FLOW CHART FOR SUBROUTINE SOILCO (cont.)

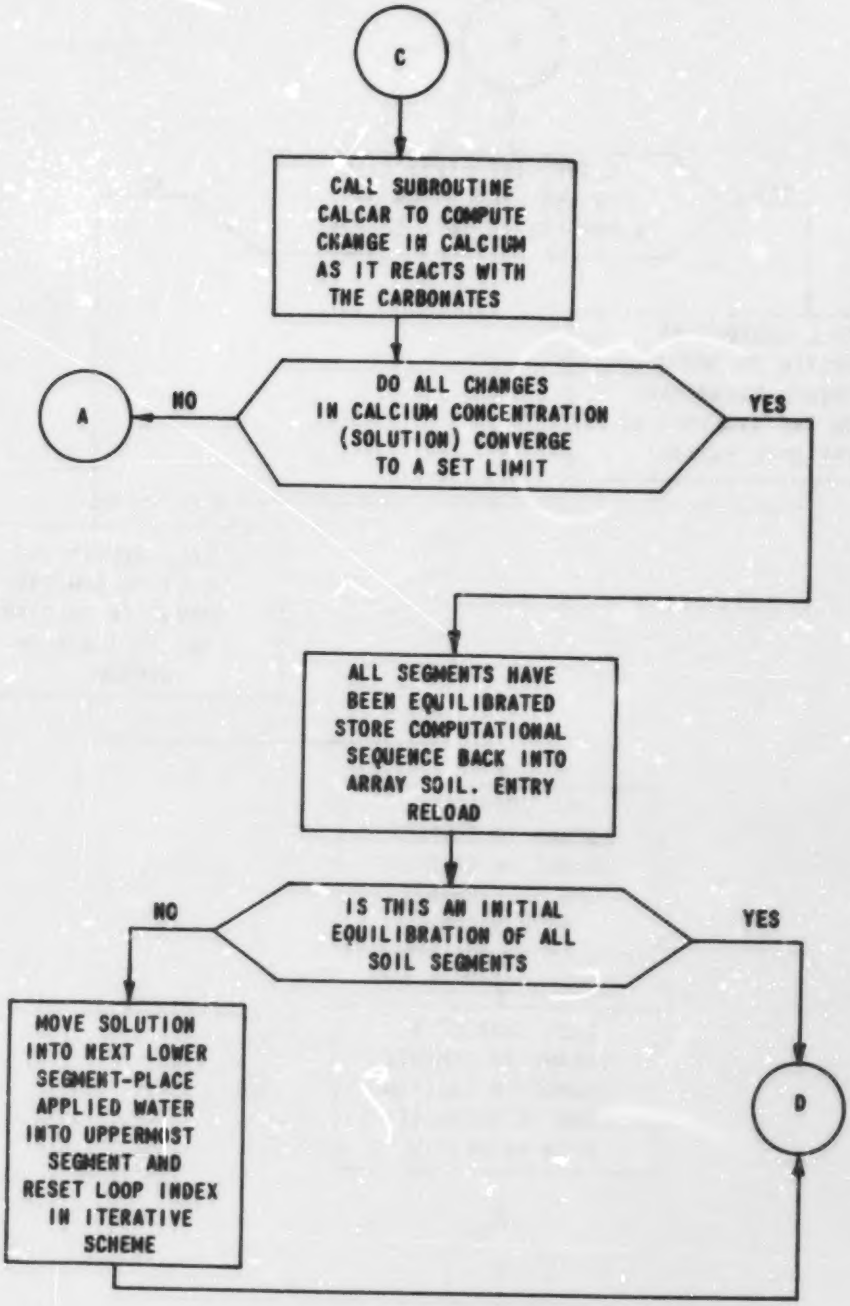

C
CALL SUBROUTINE CALCAR TO COMPUTE CKANGE IN CALCIUM AS IT REACTS WITH THE CARBONATES
DO ALL CHANGES IN CALCIUM CONCENTRATION (SOLUTION) CONVERGE TO A SET LIMIT
NO
A
YES
ALL SEGMENTS HAVE BEEN EQUILIBRATED STORE COMPUTATIONAL SEQUENCE BACK INTO ARRAY SOIL. ENTRY RELOAD
IS THIS AN INITIAL EQUILIBRATION OF ALL SOIL SEGMENTS
NO
YES
MOVE SOLUTION INTO NEXT LOWER SEGMENT-PLACE APPLIED WATER INTO UPPERMOST SEGMENT AND RESET LOOP INDEX IN ITERATIVE SCHEME
D

FIGURE 37

FLOW CHART FOR SUBROUTINE SOILCO (cont.)

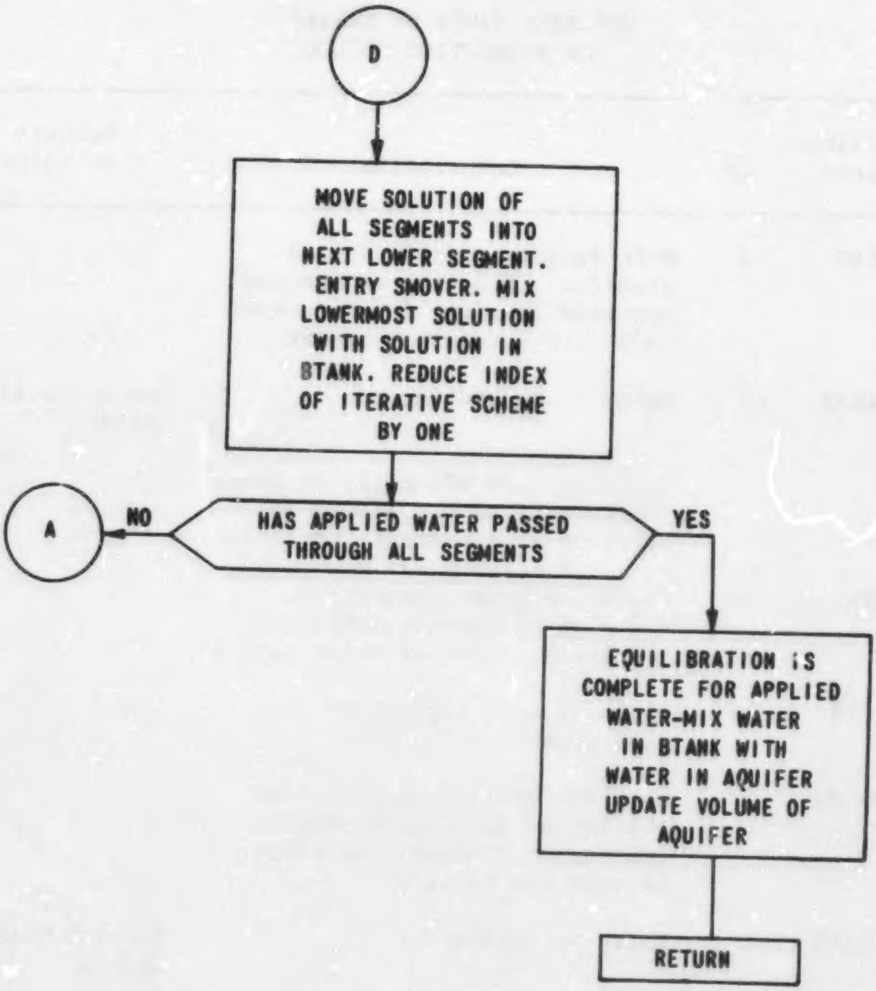

D
MOVE SOLUTION OF ALL SEGMENTS INTO NEXT LOWER SEGMENT. ENTRY SMOVER. MIX LOWERMOST SOLUTION WITH SOLUTION IN BTANK. REDUCE INDEX OF ITERATIVE SCHEME BY ONE
A
NO
HAS APPLIED WATER PASSED THROUGH ALL SEGMENTS
YES
EQUILIBRATION IS COMPLETE FOR APPLIED WATER-MIX WATER IN BTANK WITH WATER IN AQUIFER UPDATE VOLUME OF AQUIFER
RETURN

FIGURE 38

Table 12

VARIABLE NAMES OR ARRAYS FOR SUBROUTINE SOILCO

Variable name	C*	Description	Remarks or units
BDENS	C	Bulk density of soil = 1.33 grams/cm^3 (function of assumed particle density of 2.66 grams/cm^3). Can vary with segment.	
CALCAR		Entry to subroutine	See subroutine CALCAR
CA		Computational aid array to store concentrations of calcium in solution as convergent variable	
CATEX	C	Cation exchange capacity in units of milliequivalents per 100 grams. Can vary with segment.	
DEPTH	C	Depth of soil segment in centimeters	
EPSLON		Absolute difference of concentration of calcium in solution as exchanges and reactions converge to some set limit	
EXCAMG		Entry to subroutine	See subroutine EXCAMG
EXCANA		Entry to subroutine	See subroutine EXCANA
EXTRAC		Ratio of water to soil as used in soil analysis (laboratory)	
FRSTIM		Entry to subroutine	See subroutine FRSTIM
GYPEX		Entry to subroutine	See subroutine GYPEX

Table 12 - Continued

Variable name	C*	Description	Remarks or units
IFIR		Call index to this subroutine	
I		Loop index	
ISW		Switch used to determine state of iterative scheme as simulation of waters percolating through soil column continues	
ITER		Iteration counter for iterative scheme used balancing each soil segment	
IW		Write unit designation	
J		Loop index	
KNODE		Node index	
K		Loop index for iterative scheme	
KV		Loop limit	
KWATER		Counter for applied waters percolated through soil column	
L		Loop index	
MAX		Loop limit (maximum)	
MIN		Loop limit (minimum)	
NCT		Counter used for each equilibration	
NSEGS		Number of segments in soil column	
PRATIO		Moisture content in percent (gravimetric)	
RELOAD		Entry to subroutine	See subroutine SETUP

Table 12

Variable name	C*	Description	Remarks or units
SEGVOL	C	Volume of water in segment in milliliters	
SETUP		Entry to subroutine	See subroutine SETUP
SMOVER		Entry to subroutine	See subroutine SETUP
WRATIO		Moisture content-ratio of weight of water to weight of soil	

SUBROUTINE SETUP

This subroutine was designed to simplify the transfer of data from the permanent storage array "SOIL" to a transient set of variable names used in the computational mode. The subroutine has three entries including the main entry. The labels assigned to each entry are indicative of the type function performed.

The argument list consists of the node index, the soil segment sequence, the number of segments in the soil column, and a switch index.

The main entry SETUP is used to convert units of input data of the initial soil analysis to the computational units. This conversion is only made once for each soil segment of each soil column for each input; i.e., when switch index is set to zero. Subsequent to the conversion the data from the "SOIL" array is loaded into the computational variable name sequence, and from this point on all data in the "SOIL" array will be in the units required for computation.

A call to the entry SETUP is made from the monitor subroutine SOILCO as is the case for the other two entries.

Entry SMOVER simulates the movement of the solution down through the soil segment (piston effect). The first step is the conversion of the concentrations of the constituents in the solution of the lowermost segments to parts per million and mixed (linear) with the solution of the symbolically labeled BTANK. The second step is the transfer of the solution from each of the soil segments to the next lower soil segment. During the first transfer the applied water is transferred to the uppermost segment.

Entry RELOAD is called after all segments have been equilibrated following each move. Data is transferred back into the array "SOIL" from the computational variable name sequence.

The flow chart for this subroutine is shown on Figure 39. The variable names or data arrays are shown in Table 13.

FLOW CHART FOR SUBROUTINE SETUP

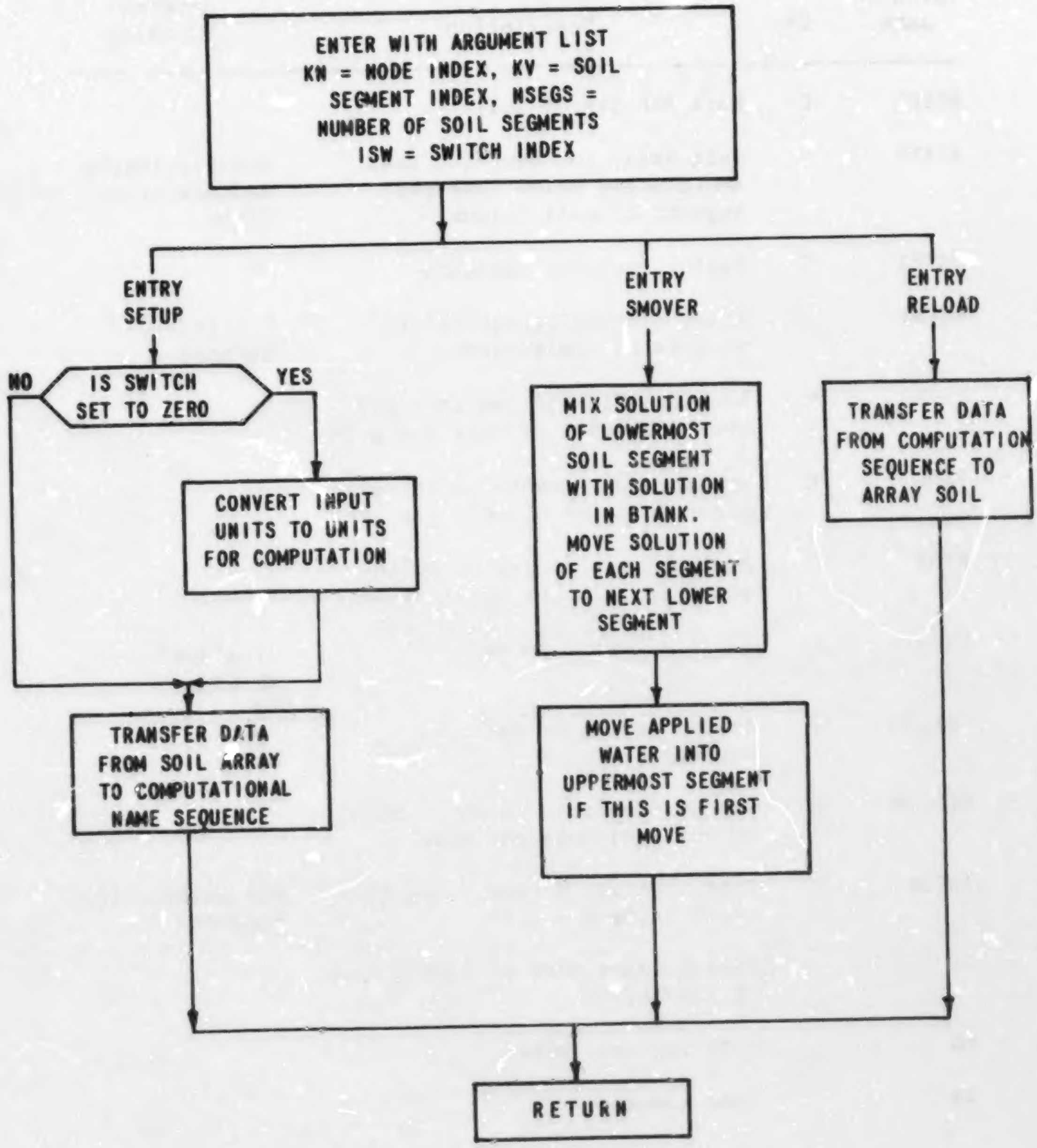

ENTER WITH ARGUMENT LIST
KN = NODE INDEX, KV = SOIL SEGMENT INDEX, NSEGS = NUMBER OF SOIL SEGMENTS
ISW = SWITCH INDEX
ENTRY SETUP
ENTRY SMOVER
ENTRY RELOAD
IS SWITCH SET TO ZERO
NO
YES
CONVERT INPUT UNITS TO UNITS FOR COMPUTATION
TRANSFER DATA FROM SOIL ARRAY TO COMPUTATIONAL NAME SEQUENCE
MIX SOLUTION OF LOWERMOST SOIL SEGMENT WITH SOLUTION IN BTANK. MOVE SOLUTION OF EACH SEGMENT TO NEXT LOWER SEGMENT
MOVE APPLIED WATER INTO UPPERMOST SEGMENT IF THIS IS FIRST MOVE
TRANSFER DATA FROM COMPUTATION SEQUENCE TO ARRAY SOIL
RETURN

FIGURE 39

Table 13

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE SETUP

Variable name	C*	Description	Remarks or units
BDENS	C	Bulk density of soil	
BTANK	C	Data array for symbolic tank immediately below lowermost segment of soil column	See previously defined array BTANK
CATEX	C	Cation exchange capacity	
EQVWT		Array containing equivalent weights of constituents	Previously defined
EXCA	C	Exchangeable calcium in solid phase in units of mols per gram	
EXMG	C	Exchangeable magnesium in solid phase in units of mols per gram	
EXNA	C	Exchangeable sodium in solid phase in units of mols per gram	
EXTRAC	C	Ratio of water to soil	Previously defined
GRTANK	C	Array containing data for aquifer	Previously defined
GYPSUM	C	Gypsum dihydrate ($CaSO_4 \cdot 2H_2O$) in units of mols per gram	
INTER	C	Intercept for K' where $\log K' = -1.68 \cdot \log M - 4.46$	See mathematical appendix
ISW		Switch index used to denote mode of simulation	
KG		Soil segment index	
KN		Node index	

Table 13 - Continued

Variable name	C*	Description	Remarks or units
KP		Loop index	
KR		Loop index	
K		Loop index	
KV		Soil segment index	
L		Loop index	
NSEGS		Number of soil segments in a soil column	
SEGVOL	C	Volume of water in soil segment in milliliters	
SLCA	C	Concentration of calcium in solution in mols per liter	
SLCL	C	Concentration of chloride in solution in mols per liter	
SLCO3	C	Concentration of carbonate in solution in mols per liter	
SLHCO3	C	Concentration of bicarbonate in solution in mols per liter	
SLIME	C	Indicator designating presence of lime in soil	
SLNA	C	Concentration of sodium in solution in mols per liter	
SLNO3	C	Concentration of nitrate in solution in mols per liter	
SLSO4	C	Concentration of sulfate in solution in mols per liter	
SOIL	C	Array containing data related to the simulation of a soil column	See data array SOIL

Table 13 - Continued

Variable name	C*	Description	Remarks or units
TTANK	C	Array containing data for applied water in ponding pool	See previously defined data array TTANK
UCASO4	C	Concentration of undissociated calcium sulfate in mols per liter	
UMGSO4	C	Concentration of undissociated magnesium sulfate in mols per liter	
VALNCE		Array containing valence of constituents	See data array VALNCE

ARRAY SOIL (20,10,21)

SOIL (J,K,1) = Concentration of calcium in solution in mols per liter

SOIL (J,K,2) = Concentration of magnesium in solution in mols per liter

SOIL (J,K,3) = Concentration of sodium in solution in mols per liter

SOIL (J,K,4) = Concentration of chloride in solution in mols per liter

SOIL (J,K,5) = Concentration of sulfate in solution in mols per liter

SOIL (J,K,6) = Concentration of bicarbonate in solution in mols per liter

SOIL (J,K,7) = Concentration of carbonate in solution in mols per liter

SOIL (J,K,8) = Concentration of nitrate in solution in mols per liter

Table 13 - Continued

ARRAY SOIL (20,10,21) - continued

SOIL (J,K,9)	= Extract ratio from initial soil analysis	Weight of water/weight of soil
SOIL (J,K,10)	= Volume of water in soil segment in units of milliliters	
SOIL (J,K,11)	= Cation exchange capacity in solid phase (soil) in units of mols per gram	
SOIL (J,K,12)	= Gypsum dihydrate in units of mols per gram	
SOIL (J,K,13)	= Lime ($CaCO_3$) indicator in solid phase	1.0=present 0.0=not present
SOIL (J,K,14)	= Bulk density of soil in units of grams per cubic centimeter	
SOIL (J,K,15)	= Length of soil segment in centimeters	
SOIL (J,K,16)	= Exchangeable calcium in solid phase in units of mols per gram	
SOIL (J,K,17)	= Exchangeable magnesium in solid phase in units of mols per gram	
SOIL (J,K,18)	= Exchangeable sodium in solid phase in units of mols per gram	
SOIL (J,K,19)	= Undissociated calcium sulfate in solution in units of mols per liter	
SOIL (J,K,20)	= Undissociated magnesium sulfate in solution in units of mols per liter	
SOIL (J,K,21)	= Intercept for K' (see mathematical appendix)	

J = Node index K = soil segment index

Table 13 - Continued

ARRAY VALNCE (8)

VALNCE (1) = Valence of calcium = 2
VALNCE (2) = Valence of magnesium = 2
VALNCE (3) = Valence of sodium = 1
VALNCE (4) = Valence of chloride = 1
VALNCE (5) = Valence of sulfate = 2
VALNCE (6) = Valence of bicarbonate = 1
VALNCE (7) = Valence of carbonate = 2
VALNCE (8) = Valence of nitrate = 1

SUBROUTINE FRSTIM

This subroutine is called only once per soil segment per soil column. The overall simulation of the soil column will accommodate ten segments per soil column.

The argument list consists of the node index, the segment index, and the write unit designation.

The subroutine is used to compute the concentrations of the various constituents such as calcium, magnesium, sodium, and the dissociated calcium sulfate and magnesium sulfate all in the solution phase.

The exchangeable cations of the soil or solid phase are also computed in this subroutine.

The subroutine is actually the equilibration of each soil segment using the data from the initial soil analysis (laboratory). The derivation of the polynomials as used in this subroutine is included in the mathematical appendix.

The logic used in the subroutine is straightforward; a flow chart is shown in Figure 40. The variable names or data arrays are shown in Table 14.

FLOW CHART FOR SUBROUTINE FRSTIM

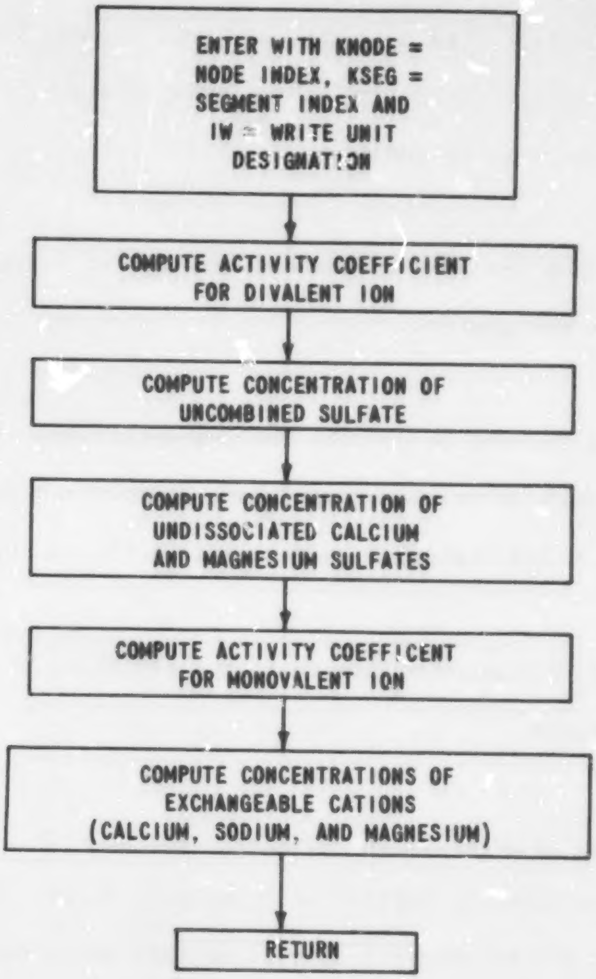

ENTER WITH KNODE = NODE INDEX, KSEG = SEGMENT INDEX AND IW = WRITE UNIT DESIGNATION
COMPUTE ACTIVITY COEFFICIENT FOR DIVALENT ION
COMPUTE CONCENTRATION OF UNCOMBINED SULFATE
COMPUTE CONCENTRATION OF UNDISSOCIATED CALCIUM AND MAGNESIUM SULFATES
COMPUTE ACTIVITY COEFFICENT FOR MONOVALENT ION
COMPUTE CONCENTRATIONS OF EXCHANGEABLE CATIONS (CALCIUM, SODIUM, AND MAGNESIUM)
RETURN

FIGURE 40

Table 14

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE FRSTIM

Variable name	C*	Description	Remarks or units
BDENS	C	Bulk density of soil	
CA		An array used as a computational aid in passing coefficients of polynomials	
CATEX	C	Cation exchange capacity	
CONST		Computational aid	
EXCA	C	Exchangeable calcium in solid phase	
EXMG	C	Exchangeable magnesium in solid phase	
EXNA	C	Exchangeable sodium in solid phase	
FSO4		Computation aid that represents the uncombined sulfate	
GAMMA1		Activity coefficient for a monovalent ion	
GAMMA2		Activity coefficient for a divalent ion	
GAMMA		Entry to Function GAMMA	See function GAMMA
GSQR		(Activity coefficient for a divalent ion) squared	
IW		Write unit designation	
KNODE		Node index	
K		Loop index	

Table 14 - Continued

Variable name	C*	Description	Remarks or units
KSEG		Segment index	
MOLE		Six alpha characters used in function ROOT to designate calling subroutine	
ROOT		Entry to function ROOT	See previously defined subroutine ROOT
SLCA		Concentration of calcium in solution in mols per liter	
SLMG		Concentration of magnesium in solution in mols per liter	
SLNA		Concentration of sodium in solution in mols per liter	
SLSO4		Concentration of sulfate in solution in mols per liter	
TECA		Thermodynamic equilibrium constant for calcium sulfate. (See Reference 1.)	
TECMG		Thermodynamic equilibrium constant for magnesium sulfate.(See Reference 1.)	
TESTA		Convergence term for use in function ROOT	
UCASO4		Concentration of undissociated calcium sulfate in solution	
UMGSO4		Concentration of undissociated magnesium sulfate in solution	
XMAX		Maximum limit of a root	
XMIN		Minimum limit of a root (real) in a definite range	

SUBROUTINE FRSTIM

REFERENCES

1. Garrels, Robert, M. and Christ, Charles, L., "Solutions, Minerals, and Equilibria," Harper and Row, 1965.

SUBROUTINE GYPEX

This subroutine is used to simulate the state of gypsum dihydrate during the equilibrium process or the exchanges between the solution and solid phase (soil). Also simulated (computed) are the changes in concentration of the ion pairs calcium and magnesium sulfates (undissociated).

The argument list consists of the node index, segment index, the write unit designation, and the moisture content in percent.

The logic and derivation of the equations used in this subroutine are included in the mathematical appendix.

The concentration of calcium in solution at the completion of the computations contained in this subroutine is stored and used as part of the convergence criteria in the soil column simulation of the equilibrium process.

The basic functions of this subroutine are indicated by the flow chart shown on Figure 41. The variable names or data arrays are shown in Table 15.

FLOW CHART FOR SUBROUTINE GYPEX

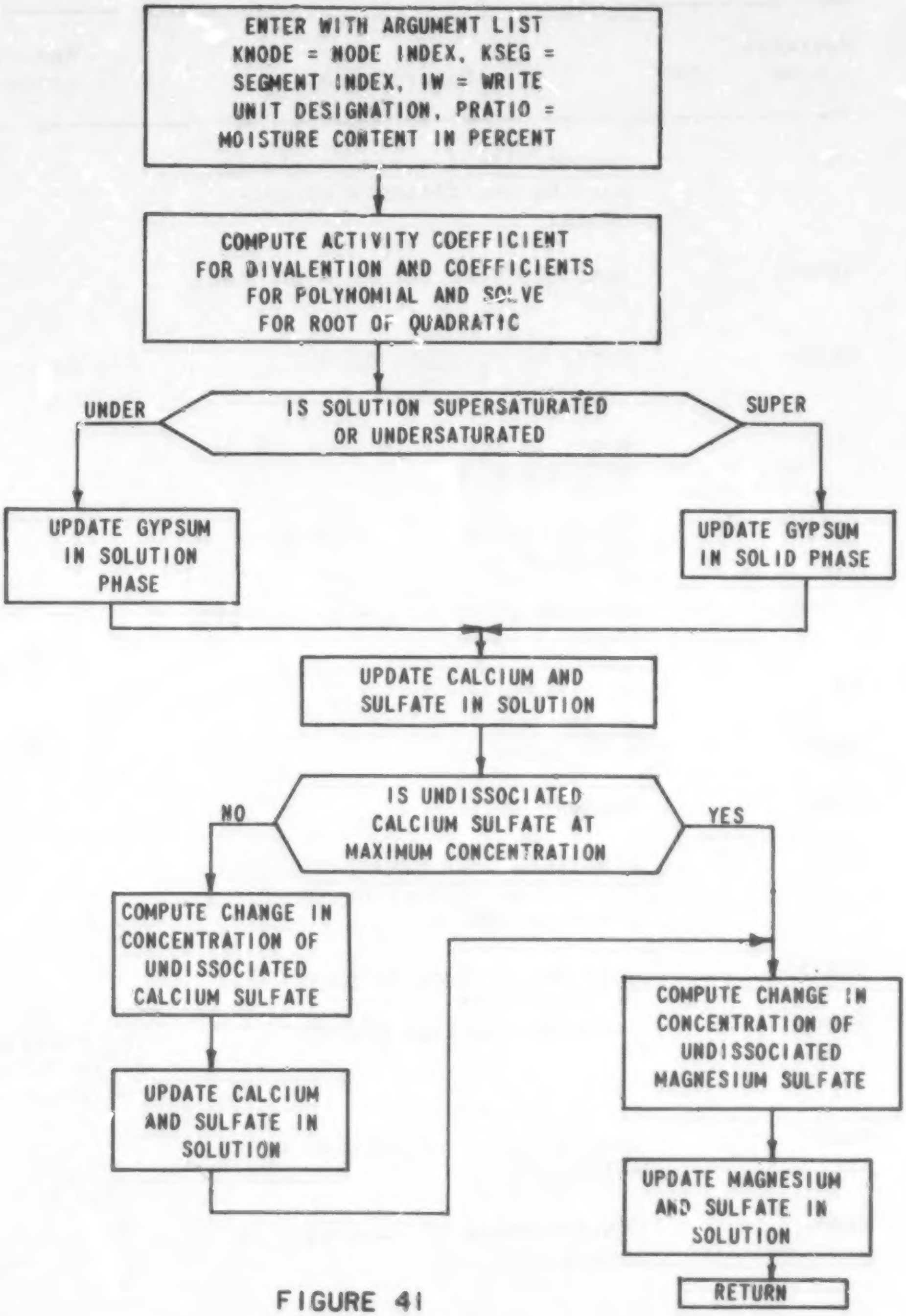

ENTER WITH ARGUMENT LIST KNODE = NODE INDEX, KSEG = SEGMENT INDEX, IW = WRITE UNIT DESIGNATION, PRATIO = MOISTURE CONTENT IN PERCENT
COMPUTE ACTIVITY COEFFICIENT FOR DIVALENTION AND COEFFICIENTS FOR POLYNOMIAL AND SOLVE FOR ROOT OF QUADRATIC
UNDER
IS SOLUTION SUPERSATURATED OR UNDERSATURATED
SUPER
UPDATE GYPSUM IN SOLUTION PHASE
UPDATE GYPSUM IN SOLID PHASE
UPDATE CALCIUM AND SULFATE IN SOLUTION
NO
IS UNDISSOCIATED CALCIUM SULFATE AT MAXIMUM CONCENTRATION
YES
COMPUTE CHANGE IN CONCENTRATION OF UNDISSOCIATED CALCIUM SULFATE
UPDATE CALCIUM AND SULFATE IN SOLUTION
COMPUTE CHANGE IN CONCENTRATION OF UNDISSOCIATED MAGNESIUM SULFATE
UPDATE MAGNESIUM AND SULFATE IN SOLUTION
RETURN

FIGURE 41

Table 15

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE GYPEX

Variable name	C*	Description	Remarks or units
CA		Computational array to aid in passing coefficients of polynomial	
GAMMA2		Activity coefficient - divalent ion	
GAMMA		Entry to Function GAMMA	See Function GAMMA
GSQR		Activity coefficient of divalent ion squared	
GYPSOL		Concentration of gypsum in solution	
GYPSUM		Concentration of gypsum in solid phase	
IW		Write unit designation	
KNODE		Node index	
KSEG		Segment index	
MOLE		Six alpha character designation of calling subroutine for function ROOTWO	
PRATIO		Moisture content in percent (gravimetric)	
ROOTWO		Entry to function ROOTWO	See previously defined function ROOTWO
SLCA		Concentration of calcium in solution	
SLMG		Concentration of magnesium in solution	

Table 15- Continued

Variable name	C*	Description	Remarks or units
SLSO4		Concentration of sulfate in solution	
UCASO4		Concentration of undissociated calcium sulfate in solution	
UMGSO4		Concentration of undissociated magnesium sulfate in solution	
W		Computational aid	
X		Root of polynomial	
Y		Gypsum in solution	

SUBROUTINE EXCANA

This subroutine simulates the exchange between calcium and sodium in both the solution and solid phases. The mathematical formulation of this exchange is included in the mathematical appendix and has as a basis the Gapon exchange equation.

The argument list consists of the node index, the segment index, the write unit designation, and the moisture content in percent.

Experience has indicated that the exchange coefficient used in this portion of the simulation is highly sensitive. The exchange coefficient used in this subroutine is set at 0.707 (see Reference 1); and on the basis of several applications, evidence is available that strongly suggests a much higher exchange coefficient is required. This evidence also suggests that the exchange coefficient is highly dependent upon the soil type and varies within a wide range from soil type to soil type.

An indication that the exchange coefficient is incorrect can be detected by an examination of the net change in the calcium and sodium concentrations as the equilibrium process passes through this portion of the simulation. It would be helpful if experimental data were available for comparison of the predicted and experimental results to better establish a range of exchange coefficients for each general type soil. However, the insertion of different values of the exchange coefficient can easily be accomplished within the model structure without any modification to the computer program.

The concentration of calcium in solution is also the convergence variable in this portion of the overall soil column simulation.

A flow chart of this subroutine is shown on Figure 42. The variable names or data arrays are shown in Table 16.

FLOW CHART FOR SUBROUTINE EXCANA

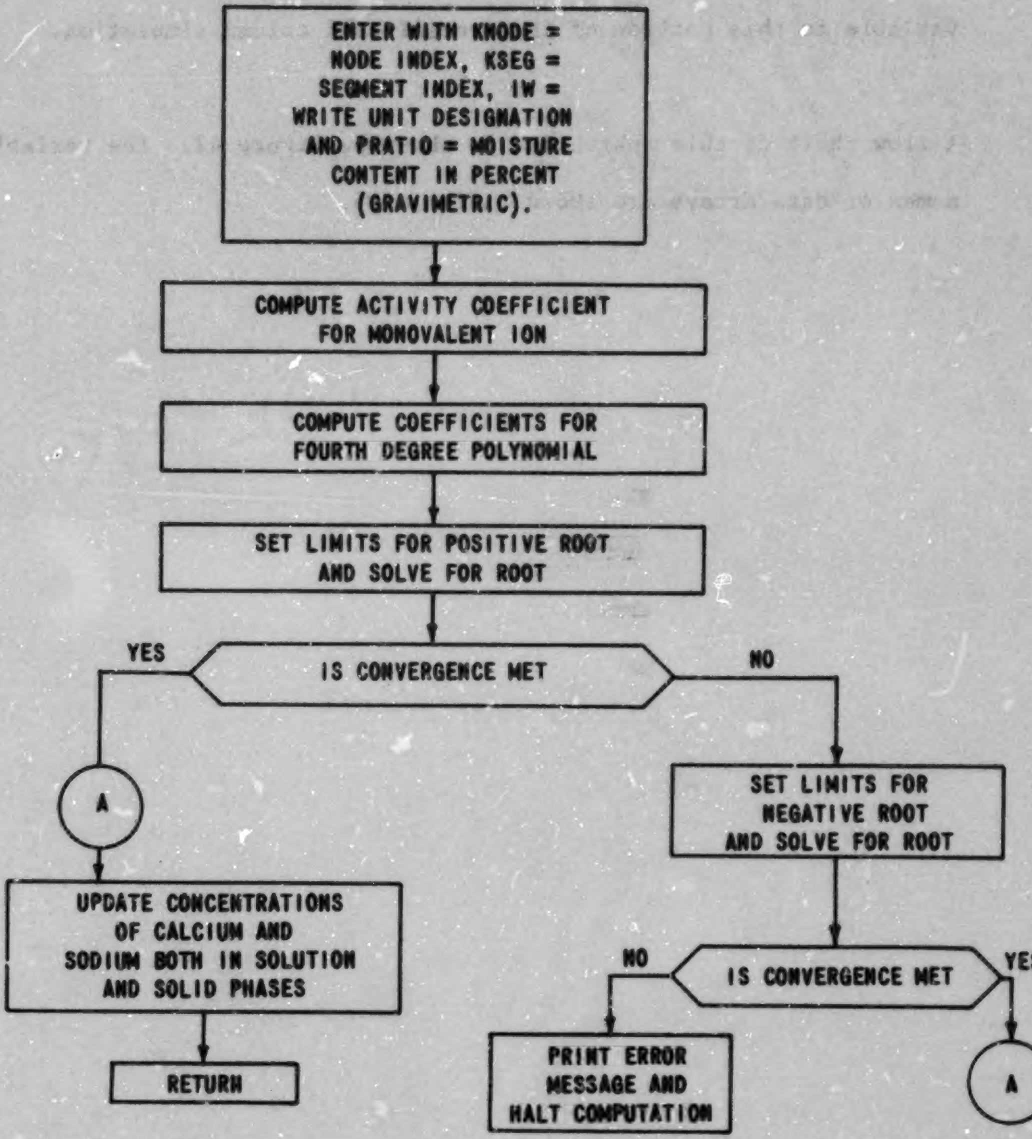

ENTER WITH KNODE = NODE INDEX, KSEG = SEGMENT INDEX, IW = WRITE UNIT DESIGNATION AND PRATIO = MOISTURE CONTENT IN PERCENT (GRAVIMETRIC).
COMPUTE ACTIVITY COEFFICIENT FOR MONOVALENT ION
COMPUTE COEFFICIENTS FOR FOURTH DEGREE POLYNOMIAL
SET LIMITS FOR POSITIVE ROOT AND SOLVE FOR ROOT
YES
IS CONVERGENCE MET
NO
A
SET LIMITS FOR NEGATIVE ROOT AND SOLVE FOR ROOT
UPDATE CONCENTRATIONS OF CALCIUM AND SODIUM BOTH IN SOLUTION AND SOLID PHASES
NO
IS CONVERGENCE MET
YES
RETURN
PRINT ERROR MESSAGE AND HALT COMPUTATION
A

FIGURE 42

Table 16

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE EXCANA

Variable name	C*	Description	Remarks or units
BETA		Conversion factor used to convert moles per gram to units mols per liter	
BETA2		BETA as described above squared	
CA		Computational array to aid in passing coefficients of polynomials	
CONST		A constant used in the argument list for function ROOT (not required in this subroutine)	
DEX		Exchange coefficient	
DEX2		Exchange coefficient DEX squared	
EXCA	C	Exchangeable calcium in solid phase	
EXNA	C	Exchangeable sodium in solid phase	
GAMMA1		Activity coefficient for a monovalent ion	
GSQR		(Activity coefficient GAMMA1) squared	
ISW		Computational aid used as a switching device in changing limits of desired root	
IW		Write unit designation	
KNODE		Node index	
K		Loop index	

Table 16 - Continued

Variable name	C*	Description	Remarks or units
KSEG		Segment index	
MOLE		Six alpha characters used in function ROOT to designate calling subroutine	
SLCA	C	Concentration of calcium in solution in mols per liter	
SLNA	C	Concentration of sodium in solution in mols per liter	
TESTA		Convergence term for use in function ROOT	
T		Array used as a computational aid	
XMAX		Maximum limit of a root	
XMIN		Minimum limit of a root (real) in a definite range	
X		Root of polynomial or change in calcium in mols per gram	

SUBROUTINE EXCANA

REFERENCES

1. Dutt, Gordon R., Shaffer, Marvin J., and Moore, William J., "Computer Simulation Model of Dynamic Bio-Physicochemical Processes in Soils," Technical Bulletin 196, Agricultural Experiment Station, The University of Arizona, October 1972.

SUBROUTINE EXCAMG

This subroutine is used to simulate the exchange between calcium and magnesium in both the solution and solid phases. The mathematical formulation of this exchange is included in the mathematical appendix.

The argument list consists of the node index, the segment index, the write unit designation, and the moisture content in percent (gravimetric).

The exchange coefficient which has a numerical value of 0.67 (see Reference 1) is generally accepted and has not presented any problems in the application of this portion of the simulation.

The variable names or arrays are shown in Table 17.

The concentration of calcium in solution at the completion of the computations contained in this subroutine is stored and used as part of the convergence criteria in the soil column simulation of the equilibrium process.

Table 17

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE EXCAMG

Variable name	C*	Description	Remarks or units
BETA		Conversion factor used to convert mols per gram to units of mols per liter	
CA		Computational array to aid in passing coefficients of polynomials	
DEX		Exchange coefficient	
EXCA	C	Exchangeable calcium in solid phase	
EXMG	C	Exchangeable magnesium in solid phase	
KNODE		Node index	
KSEG		Segment index	
MOLE		Six alpha characters used in function ROOTWO to designate calling subroutine	
PRATIO		Moisture content	
ROOTWO		Entry to function ROOTWO	See previously defined ROOTWO
SLCA	C	Concentration of calcium in solution in mols per liter	
SLMG	C	Concentration of magnesium in solution in mols per liter	
X		Root of polynomial or change in calcium and magnesium in mols per gram	

SUBROUTINE CALCAR

This subroutine is used to simulate the reaction of calcium with the carbonates. The mathematical formulation of these reactions is included in the mathematical appendix.

The argument list consists of the node index, the segment index, the write unit designation, and the moisture content in percent (gravimetric).

The initial input of data for the soil column simulation contains an indicator signifying the presence or lack of presence of lime ($CaCO_3$) in the soil or solid phase. Then intercept for the relationship of K' is either computed or set as a constant dependent upon the lime condition. The significance of K' is explained in the mathematical appendix. The intercept is only computed once per segment per soil column per run.

The concentration of calcium in solution at the completion of the computations contained in this subroutine is stored and used as part of the convergence criteria in the soil column simulation of the equilibrium process.

The flow chart for this subroutine is shown on Figure 43, and the variable names or arrays are shown in Table 18.

FLOW CHART FOR SUBROUTINE CALCAR

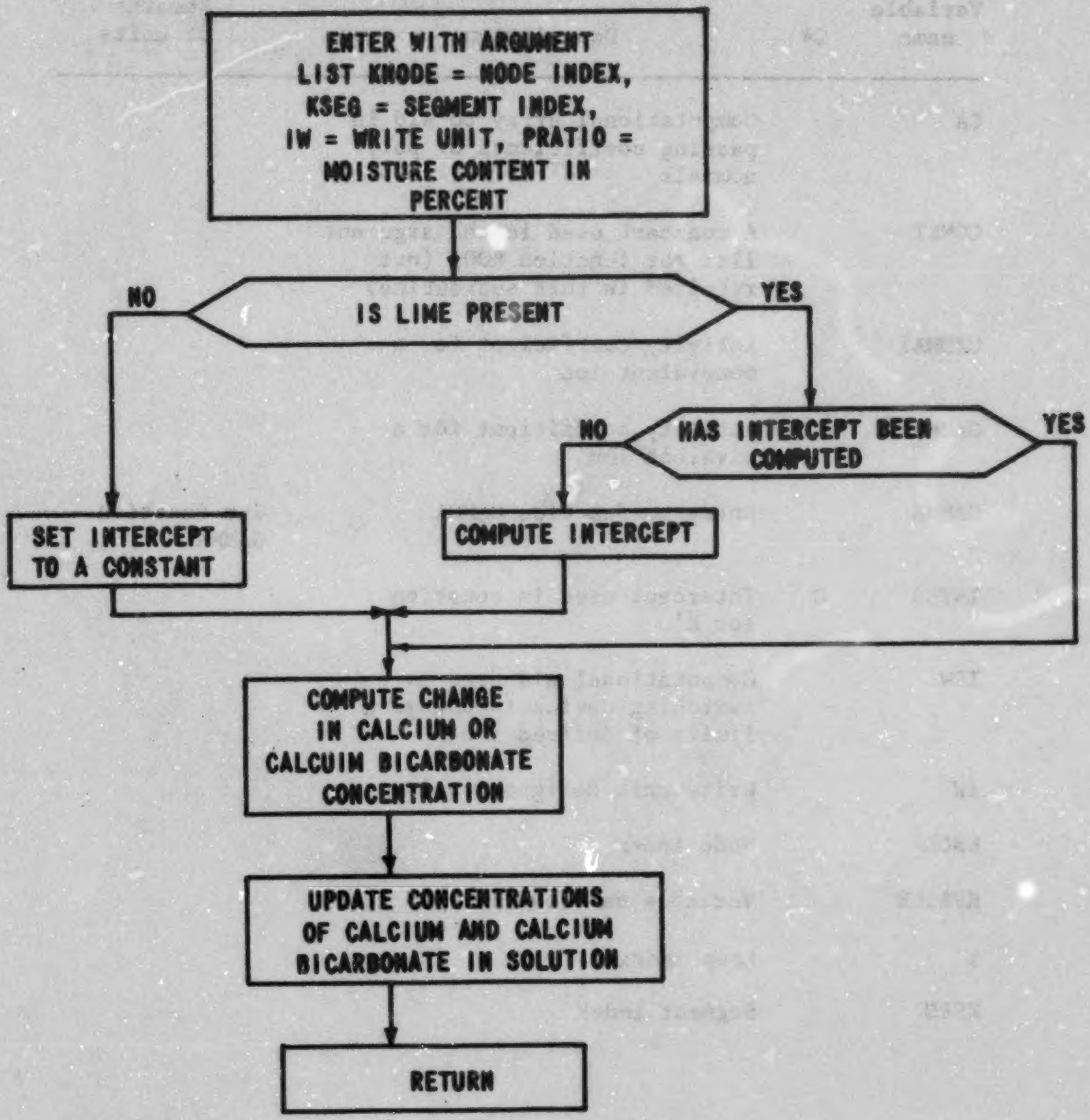

ENTER WITH ARGUMENT LIST KNODE = NODE INDEX, KSEG = SEGMENT INDEX, IW = WRITE UNIT, PRATIO = MOISTURE CONTENT IN PERCENT
NO
IS LIME PRESENT
YES
NO
HAS INTERCEPT BEEN COMPUTED
YES
SET INTERCEPT TO A CONSTANT
COMPUTE INTERCEPT
COMPUTE CHANGE IN CALCIUM OR CALCUIM BICARBONATE CONCENTRATION
UPDATE CONCENTRATIONS OF CALCIUM AND CALCIUM BICARBONATE IN SOLUTION
RETURN

FIGURE 43

Table 18

VARIABLE NAMES OR DATA ARRAYS FOR SUBROUTINE CALCAR

Variable name	C*	Description	Remarks or units
CA		Computational array to aid in passing coefficients of polynomials	
CONST		A constant used in the argument list for function ROOT (not required in this subroutine)	
GAMMA1		Activity coefficient for a monovalent ion	
GAMMA2		Activity coefficient for a divalent ion	
GAMMA		Entry to function GAMMA	See function GAMMA
INTER	C	Intercept used in equation for K'	
ISW		Computational aid used as a switching device in changing limits of desired root	
IW		Write unit designation	
KNODE		Node index	
KPRIME		Variable name for K'	
K		Loop index	
KSEG		Segment index	

Table 18 - Continued

Variable name	C*	Description	Remarks or units
MOLE		Six alpha characters used in function ROOT to designate calling subroutine	
PRATIO		Moisture content in percent (gravimetric)	
ROOT		Entry to function ROOT	
SLCA	C	Concentration of calcium in solution in mols per liter	
SLHCO3	C	Concentration of sodium bicarbonate in solution in mols per liter	
SLIME	C	Indicator to designate presence of lime in soil	
TEMP		Computational aid	
TESTA		Convergence term for use in function ROOT	
XMAX		Maximum limit of root	
XMIN		Minimum limit of root (real) in a definite range	
X		Change in concentration of calcium and bicarbonate in solution in units of mols per liter	

SUBROUTINE CALCAR

REFERENCES

1. Dutt, Gordon, R., "Prediction of the Concentration of Solutes in Soil Solutions for Soil Systems Containing Gypsum and Exchangeable Ca and Mg," Soil Science Society of America, Proceedings, Volume 26, Number 4, July-August 1962, pages 341-343.

SUBROUTINE SCRIBE

This routine is used to output the values of pertinent parameters of the soil-water equilibration.

The argument list consists of on the write unit designation.

The units of output are those in the computational mode. This routine is an excellent diagnostic tool in the overall soil column simulation.

The variable names have all been previously defined.

FUNCTION GAMMA

This subroutine is used to compute the activity coefficient of a mono or divalent ion. The mathematical formulation for this subroutine is included in the mathematical appendix.

The argument "KVAL" represents the valence of ion.

Mathematical Appendix of Soil Column Simulation

Activity coefficient - Gamma (γ)

Debye-Hückel theory states that:

$$\mathrm{Log}_{10}(\gamma) = \frac{-\lambda Z^2 \sqrt{u}}{1 + \beta \sqrt{u}}$$

where:

λ and β are temperature constants and at 27° C or 49° F,

$\lambda = 0.509$, $\beta = 1.00$

u = ionic strength

Z = valence of ion species in solution

Substitution of constants for λ and β, and changing from Log_{10} to Log_e, where $\mathrm{Log}_e\ (10) = 2.30259$, then:

$$\mathrm{Log}_e\ (\gamma) = \frac{-0.509\ (2.30259)\ Z^2 \sqrt{u}}{1 + \sqrt{u}}$$

taking logarithms of both sides -

$$\gamma = e^{\frac{-1.17201\ Z^2 \sqrt{u}}{1 + \sqrt{u}}}$$

where: ionic strength $= u = 1/2 \sum_{i=1}^{i=n} C_i Z_i^{\,2}$

where: C_i = concentration of i_{th} ion species in solution in units of moles per liter

n = number of ion species in solution

Computation of concentration of undissociated calcium sulfate ($CaSO_4^\circ$) in units of moles per liter in terms of C_{SO_4}

Begin derivation of an equation with one unknown. Let unknown equal concentration of the uncombined sulfate -

$$\text{Let - } C_{SO_{4T}} = C_{SO_4} + C_{CaSO_4} + C_{MgSO_4} \tag{1}$$

where: $C_{SO_{4T}}$ = concentration of sulfate in soil extract in units of moles per liter (total)

C_{SO_4} = concentration of uncombined sulfate (sulfate ion) in units of moles per liter

C_{CaSO_4} = concentration of sulfate that combines with calcium to form $CaSO_4^\circ$ in solution in units of moles per liter

C_{MgSO_4} = concentration of sulfate that combines with magnesium to form $MgSO_4^\circ$ in solution in units of moles per liter

In the use of equation (1) it becomes necessary to find expressions for C_{CaSO_4} and C_{MgSO_4} in terms of C_{SO_4}.

Solving for C_{CaSO_4} in terms of C_{SO_4}:

$$\text{Let - } C_{Ca_T} = C_{Ca} + C_{CaSO_4}$$

where: C_{Ca_T} = concentration of calcium in soil extract in units of moles per liter

C_{Ca} = concentration of uncombined calcium (calcium ion) in units of moles per liter

C_{CaSO_4} = concentration of calcium that combines with sulfate to form $CaSO_4^\circ$ in solution in units of moles per liter

Given the thermodynamic equilibrium constant (K_{CaSO_4}) for $CaSO_4^\circ$ as -

$$K_{CaSO_4} = \frac{a_{Ca} \cdot a_{SO_4}}{a_{CaSO_4}} \qquad (2)$$

where:

a_{Ca} = activity of calcium ion

a_{SO_4} = activity of sulfate ion

a_{CaSO_4} = activity of calcium sulfate (ion pair)

and

$$a_{Ca} = C_{Ca} \cdot \gamma_{Ca}$$

$$a_{SO_4} = C_{SO_4} \cdot \gamma_{SO_4}$$

$$a_{CaSO_4} = C_{CaSO_4} \cdot \gamma_{CaSO_4}$$

Assume $\gamma_{CaSO_4} = 1.00$

Substitution into equation (2) then

$$K_{CaSO_4} = \frac{C_{Ca} \cdot \gamma_{Ca} \cdot C_{SO_4} \cdot \gamma_{SO_4}}{C_{CaSO_4}} \qquad (3)$$

Solving for C_{Ca} using equation (3)

$$C_{Ca} = \frac{K_{CaSO_4} \cdot C_{CaSO_4}}{\gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}}$$

then: $$C_{Ca_T} = \frac{K_{CaSO_4} \cdot C_{CaSO_4}}{\gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}} + C_{CaSO_4}$$

or: $$C_{Ca_T}(\gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}) = K_{CaSO_4} \cdot C_{CaSO_4} + C_{CaSO_4}(\gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4})$$

$$= C_{CaSO_4}(K_{CaSO_4} + \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4})$$

and: $$C_{CaSO_4} = \frac{C_{Ca_T} \cdot \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}}{K_{CaSO_4} + \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}}$$

experimentally $K_{CaSO_4} = 4.9 \cdot 10^{-3}$

The expression then for C_{CaSO_4} in terms of C_{SO_4}

is

$$C_{CaSO_4} = \frac{C_{Ca_T} \cdot \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}}{4.9 \cdot 10^{-3} + \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}} \qquad (4)$$

Computation of concentration of undissociated magnesium sulfate ($MgSO_4^\circ$) in units of moles per liter in terms of C_{SO_4}

Solving for C_{MgSO_4} in terms of C_{SO_4} -

Let $C_{Mg_T} = C_{Mg} + C_{MgSO_4}$

where: C_{Mg_T} = concentration of magnesium in units of moles per liter (total)

C_{Mg} = concentration of uncombined magnesium (magnesium ion) in units of moles per liter

C_{MgSO_4} = concentration of magnesium that combines with sulfate to form $MgSO_4^\circ$ in solution in units of moles per liter

Given the thermodynamic equilibrium constant (K_{MgSO_4}) for $MgSO_4^\circ$ as -

$$K_{MgSO_4} = \frac{a_{Mg} \cdot a_{SO_4}}{a_{MgSO_4}} \qquad (5)$$

where: a_{Mg} = activity of magnesium ion

a_{SO_4} = activity of sulfate ion

a_{MgSO_4} = activity of magnesium sulfate (ion pair)

and: $a_{Mg} = C_{Mg} \cdot \gamma_{Mg}$

$a_{SO_4} = C_{SO_4} \cdot \gamma_{SO_4}$

$a_{MgSO_4} = C_{MgSO_4} \cdot \gamma_{MgSO_4}$

Assume $\gamma_{MgSO_4} = 1.00$

substitution into equation (5) then -

$$K_{MgSO_4} = \frac{C_{Mg} \cdot \gamma_{Mg} \cdot C_{SO_4} \cdot \gamma_{SO_4}}{C_{MgSO_4}} \qquad (6)$$

Solving for C_{Mg} using equation (6)

$$C_{Mg} = \frac{K_{MgSO_4} \cdot C_{MgSO_4}}{\gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}}$$

then:

$$C_{Mg_T} = \frac{K_{MgSO_4} \cdot C_{MgSO_4}}{\gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}} + C_{MgSO_4}$$

or:

$$C_{Mg_T} (\gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}) = K_{MgSO_4} \cdot C_{MgSO_4} + C_{MgSO_4} (\gamma_{mg} \cdot \gamma_{SO_4} \cdot C_{SO_4})$$

$$= C_{MgSO_4} (K_{MgSO_4} + \gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4})$$

and:

$$C_{MgSO_4} = \frac{C_{Mg_T} \cdot \gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}}{K_{MgSO_4} + \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}}$$

Experimentally $K_{MgSO_4} = 5.9 \cdot 10^{-3}$

The expression then for C_{MgSO_4} in terms of C_{SO_4} is

$$C_{MgSO_4} = \frac{C_{Mg_T} \cdot \gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}}{5.9 \cdot 10^{-3} + \gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}} \qquad (7)$$

Equations (4) and (7) are expressions of the undissociated calcium sulfate and magnesium sulfate in terms of C_{SO_4}. It now becomes necessary to solve for C_{SO_4}, which is the concentration of the uncombined sulfate (sulfate ion) in units of moles per liter substitution of equations (4) and (7) into equation (1)

$$C_{SO_{4T}} = C_{SO_4} + \frac{C_{Ca_T} \cdot \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}}{4.9 \cdot 10^{-3} + \gamma_{Ca} \cdot \gamma_{SO_4} \cdot C_{SO_4}} + \frac{C_{Mg_T} \cdot \gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}}{5.9 \cdot 10^{-3} + \gamma_{Mg} \cdot \gamma_{SO_4} \cdot C_{SO_4}}$$

$\gamma_{Ca} = \gamma_{SO_4} = \gamma_{Mg} = \gamma_2$

where: γ_2 = activity coefficient for a divalent ion.

Then:

$$C_{SO_{4T}} = C_{SO_4} + \frac{C_{Ca_T} \cdot \gamma_2^2 \cdot C_{SO_4}}{4.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4}} + \frac{C_{Mg_T} \cdot \gamma_2^2 \cdot C_{SO_4}}{5.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4}}$$

or:

$$0 = C_{SO_4} + \frac{C_{Ca_T} \cdot \gamma_2^2 \cdot C_{SO_4}}{4.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4}} + \frac{C_{Mg_T} \cdot \gamma_2^2 \cdot C_{SO_4}}{5.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4}} - C_{SO_{4T}}$$

and

$$0 = C_{SO_4}(4.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4})(5.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4}) +$$
$$C_{Ca_T} \gamma_2^2 \cdot C_{SO_4}(5.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4}) + C_{Mg_T} \cdot \gamma_2^2 \cdot C_{SO_4}$$
$$(4.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4}) - C_{SO_{4T}} (4.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4})$$
$$(5.9 \cdot 10^{-3} + \gamma_2^2 \cdot C_{SO_4})$$

expanding:

$$0 = 4.9 \cdot 10^{-3} \cdot 5.9 \cdot 10^{-3} \cdot C_{SO_4} + 5.9 \cdot 10^{-3}\, \gamma_2^2\, C^2_{SO_4} +$$

$$4.9 \cdot 10^{-3}\, \gamma_2^2 \cdot C^2_{SO_4} + \gamma_2^4 \cdot C^3_{SO_4} + 5.9 \cdot 10^{-3}\, \gamma_2^2 \cdot C_{Ca_T} \cdot C_{SO_4} +$$

$$C_{Ca_T} \cdot \gamma_2^4 \cdot C^2_{SO_4} + 4.9 \cdot 10^{-3} \cdot \gamma_2^2 \cdot C_{Mg_T} \cdot C_{SO_4} + C_{Mg_T}\, \gamma_2^4\, C^2_{SO_4} -$$

$$4.9 \cdot 10^{-3} \cdot 5.9 \cdot 10^{-3} \cdot C_{SO_{4T}} - 5.9 \cdot 10^{-3} \cdot C_{SO_{4T}} \cdot \gamma_2^2 \cdot C_{SO_4} -$$

$$4.9 \cdot 10^{-3}\, \gamma_2^2 \cdot C_{SO_{4T}} \cdot C_{SO_4} - \gamma_2^4\, C_{SO_{4T}}\, C^2_{SO_4}$$

Collecting terms:

$C^3_{SO_4}$	$C^2_{SO_4}$	C_{SO_4}	K
γ_2^4	$5.9 \cdot 10^{-3} \cdot \gamma_2^2$	$4.9 \cdot 10^{-3} \cdot 5.9 \cdot 10^{-3}$	$-4.9 \cdot 10^{-3} \cdot 5.9 \cdot 10^{-3} C_{SO_{4T}}$
	$4.9 \cdot 10^{-3} \cdot \gamma_2^2$	$5.9 \cdot 10^{-3} \cdot \gamma_2^2 \cdot C_{Ca_T}$	
	$\gamma_2^4 \cdot C_{Ca_T}$	$4.9 \cdot 10^{-3} \cdot \gamma_2^2 \cdot C_{Mg_T}$	
	$\gamma_2^4 \cdot C_{Mg_T}$	$-5.9 \cdot 10^{-3} \cdot \gamma_2^2 \cdot C_{SO_{4T}}$	
	$-\gamma_2^4 \cdot C_{SO_{4T}}$	$-4.9 \cdot 10^{-3} \cdot \gamma_2^2 \cdot C_{SO_{4T}}$	

Let $X = C_{SO_4}$ and the following third degree polynomial is developed:

$$
\begin{aligned}
0 = \gamma_2^4 X^3 + \gamma_2^2 \Big[& (5.9 \cdot 10^{-3} + 4.9 \cdot 10^{-3}) + \gamma_2^2 (C_{Ca_T} + C_{Mg_T} - C_{SO_{4T}}) \Big] X^2 \\
& + \Big[4.9 \cdot 10^{-3} . 5.9 \cdot 10^{-3} + \gamma_2^2 (5.9 \cdot 10^{-3} C_{Ca_T} + 4.9 \cdot 10^{-3} . C_{Mg_T} - \\
& \quad 5.9 \cdot 10^{-3} . C_{SO_{4T}} - 4.9 \cdot 10^{-3} C_{SO_{4T}}) \Big] X - 4.9 \cdot 10^{-3} . 5.9 \cdot 10^{-3} C_{SO_{4T}}
\end{aligned}
$$

or

$$
\begin{aligned}
0 = \gamma_2^4 X^3 + \gamma_2^2 \Big[& 1.08 \,.\, 10^{-2} + \gamma_2^2 (C_{Ca_T} + C_{Mg_T} - C_{SO_{4T}} \Big] X^2 \\
& + \Big[2.89 \cdot 10^{-5} + \gamma_2^2 (5.9 \cdot 10^{-3} C_{Ca_T} + 4.9 \cdot 10^{-3} C_{Mg_T} - \\
& \quad 1.08 \cdot 10^{-2} C_{SO_{4T}}) \Big] X - 2.89 \cdot 10^{-5} C_{SO_{4T}}
\end{aligned}
\tag{8}
$$

The real root of the above polynomial (equation (8)) must be

$$0 \leq X \leq C_{SO_{4T}}$$

The solution of equation (8) will result in the concentration of the uncombined sulfate ion SO_4 in units of moles per liter. With the value of C_{SO_4} known equations (4) and (7) can be used to determine the concentrations of the undissociated calcium sulfate ($CaSO_4^\circ$) and magnesium sulfate ($MgSO_4^\circ$).

Exchangeable cation concentrations in the solid phase

The total exchangeable cation concentrations in the solid phase are represented by the cation exchange capacity. This capacity is given as part of the initial soil analysis in units of milliequivalents per

100 grams and is converted to equivalents per gram for computational purposes. Equation (9) shows the sum of the exchangeable cations in the solid phase.

$$N_T = N_{Na} + N_{Ca} + N_{Mg} \qquad (9)$$

where: N_T = Total cation exchange capacity in units or equivalents per gram

N_{Na} = Concentration of sodium ion in the soil or solid phase in units of equivalents per gram

N_{Ca} = Concentration of calcium ion in the soil or solid phase in units of equivalents per gram

In equation (9) there are three unknowns. With the use of widely used expressions the concentrations of magnesium and sodium will be shown in terms of the concentration of calcium. An equation that is widely used for the calcium-magnesium exchange is shown below as equation (10):

$$\frac{a_{Ca}}{a_{Mg}} = K_1 \frac{N_{Ca}}{N_{Mg}} \qquad (10)$$

where: a_{Ca} = the activity of the calcium ion in solution

a_{Mg} = the activity of the magesium ion in solution

N_{Ca} and N_{Mg} have been defined above

$K_1 = 0.67$ (experimentally derived)

In a previous portion of this appendix it was shown that

$$a_{Ca} = C_{Ca} \cdot \gamma_2$$

$$a_{Mg} = C_{Mg} \cdot \gamma_2$$

where γ_2 represents activity coefficient for divalent ions.

Upon substitution into equation (10)

$$\frac{a_{Ca}}{a_{Mg}} = 0.67 \cdot \frac{N_{Ca}}{N_{Mg}} = \frac{C_{Ca} \cdot \gamma_2}{C_{Mg} \cdot \gamma_2}$$

or:

$$N_{Mg} = \frac{0.67 \cdot N_{Ca} \cdot C_{Mg}}{C_{Ca}} \qquad (11)$$

Equation (11) is an expression for the concentration of the magnesium ion in the solid phase in terms of the concentration of the calcium ion. With the use of the Gapon relationship of sodium and calcium an equation can be derived to represent the concentration of the sodium ion in the solid phase in terms of the concentration of the calcium ion.

The Gapon relationship is as follows:

$$\frac{a_{Na}}{\sqrt{a_{Ca}}} = K_2 \frac{N_{Na}}{N_{Ca}} \qquad (12)$$

where: a_{Ca} = activity of the calcium ion in solution

$= C_{Ca} \cdot \gamma_2$

a_{Na} = activity of sodium ion in solution

$= C_{Na} \cdot \gamma_1$

where γ_1 = activity coefficient for the monovalent ion

Upon substitution into equation (12)

$$\frac{a_{Na}}{\sqrt{a_{Ca}}} = K_2 \frac{N_{Na}}{N_{Ca}} = \frac{C_{Na} \cdot \gamma_1}{\sqrt{C_{Ca} \cdot \gamma_2}}$$

or:

$$N_{Na} = \frac{N_{ca} \cdot C_{Na} \cdot \gamma_1}{K_2 \sqrt{C_{Ca} \cdot \gamma_2}}$$

K_2 = 2.0 (experimentally derived)

then:

$$N_{Na} = \frac{N_{Ca} \cdot C_{Na} \cdot \gamma_1}{2.0 \sqrt{C_{Ca} \cdot \gamma_2}} \qquad (13)$$

Equation (13) is an expression for the concentration of the magnesium ion in the solid phase in terms of the calcium ion in the solid phase. Upon substitution of equations (11) and (13) into equation (9) as follows:

$$N_T = \frac{N_{Ca} \cdot C_{Na} \cdot \gamma_1}{2.0 \sqrt{C_{Ca} \cdot \gamma_2}} + N_{Ca} + \frac{0.67 \cdot N_{Ca} \cdot C_{Mg}}{C_{Ca}}$$

or:

$$N_T = N_{Ca} \left[\frac{C_{Na} \cdot \gamma_1}{2.0 \sqrt{C_{Ca} \cdot \gamma_2}} + 1.0 + \frac{0.67 \cdot C_{Mg}}{C_{Ca}} \right]$$

and:

$$N_{Ca} = \frac{N_T}{\dfrac{C_{Na} \cdot \gamma_1}{2.0 \sqrt{C_{Ca} \cdot \gamma_2}} + 1.0 + \dfrac{0.67 \cdot C_{Mg}}{C_{Ca}}} \qquad (14)$$

All the values on the right side of equation (14) can be obtained from the data of the soil extract analysis; therefore, the concentration of the calcium ion in the solid phase can be determined. After the determination of the concentration of the calcium ion equations (11) and (13) can be used to determine the concentrations of the magnesium and sodium ions, respectively, as they exist in the solid state.

Solubility of $CaCO_3$ (lime) in water

In the University of Arizona Technical Bulletin 196, dated October 1972 and titled "Computer Simulation Model of Dynamic Bio-Physicochemical Processes in Soils," the dissociation (solubility) of $CaCO_3$ is shown as:

$$CaCO_3 \rightleftharpoons Ca^{++} + CO_3^{=}$$

and the thermodynamic solubility product Ksp is given as:

$$Ksp = a_{Ca} \cdot a_{CO_3}$$

The concentration of CO_3 is a function of the CO_2 partial pressure and HCO_3^- is usually the predominant form in which CO_2 occurs in a soil-water system. Thus it is more convenient to consider the following reaction:

$$H_2CO_3 + CaCO_3 \rightleftharpoons Ca^{++} + 2H\,CO_3^-$$

where the thermodynamic equilibrium constant $K_{H_2CO_3}$ is expressed as follows:

$$K_{H_2CO_3} = \frac{a_{Ca} \cdot a^2_{HCO_3}}{a_{H_2CO_3}}$$

or

$$K_{H_2CO_3} = \frac{C_{Ca} \cdot \gamma_2 \cdot C^2_{HCO_3} \cdot \gamma_1^2}{C_{H_2CO_3} \cdot \gamma_o}$$

where γ_o = activity coefficient of unchanged species = 1.0.

$$\text{Let} \quad \frac{K_{H_2CO_3}}{\gamma_2 \cdot \gamma_1^2} = C_{Ca} \cdot C^2_{HCO_3} = \frac{K'}{\gamma_2 \cdot \gamma_1^2} \qquad (15)$$

Due to variations of CO_2 and the solubility product Ksp a relationship was developed from experimental data for the value K'. This relationship is shown in Technical Bulletin 196, page 13, equation (37) as:

$$\text{Log } K' = -1.68 \cdot \text{Log } M - 4.46 \qquad (16)$$

where M = Moisture content of soil in percent.

With equations (15) and (16) the changes in $CaCO_3$ solubility with changing moisture contents in the soils can be computed.

Let "X" = change in concentration of the divalent ion in solution in units of moles per liter

Then: $C_{Ca} = C_{Ca} + X$

$C_{HCO_3} = C_{HCO_3} + 2X$

Substitution into equation (15) -

$$\frac{K'}{\gamma_2 \cdot \gamma_1^2} = (C_{Ca} + X)\,(C_{HCO_3} + 2X)$$

$$= (C_{Ca} + X)\,(C^2_{HCO_3} + 4C_{HCO_3}\,X + 4\,X^2)$$

$$= C_{Ca} \cdot C^2_{HCO_3} + 4 \cdot C_{Ca} \cdot C_{HCO_3}\,X + 4 \cdot C_{Ca} \cdot X^2$$

$$+ C^2_{HCO_3}\,X + 4 \cdot C_{HCO_3} \cdot X^2 + 4 \cdot X^3$$

or

$$0 = C_{Ca} \cdot C^2_{HCO_3} + 4 \cdot C_{Ca} \cdot C_{HCO_3}\,X + 4 \cdot C_{Ca} \cdot X^2 + C^2_{HCO_3}\,X$$

$$+ 4 \cdot C_{HCO_3} \cdot X^2 + 4 \cdot X^3 - \frac{K'}{\gamma_2 \cdot \gamma_1^2}$$

Collecting terms:

$$\frac{X^3}{4.0} \quad \frac{X^2}{4.0\,(C_{HCO_3} + C_{Ca})} \quad \frac{X}{4.0 \cdot C_{Ca} \cdot C_{HCO_3} + C^2_{HCO_3}} \quad \frac{K}{-\frac{K'}{\gamma_2 \gamma_1^2}}$$

and

$$\gamma_2 \cdot \gamma_1^2 = \ell^{\frac{(-2.34402)(-4.68804)\sqrt{u}}{1 + \sqrt{u}}}$$

$$= \ell^{\frac{-7.030206 \cdot \sqrt{u}}{1 + \sqrt{u}}}$$

and: $0 = 4.0\,X^3 + 4.0\left(C_{HCO_3} + C_{Ca}\right)X^2 + \left(4.0\,C_{Ca}\,C_{HCO_3} + C^2_{HCO_3}\right)X - K'/\gamma_2\gamma_1^2$

Determination of change of gypsum from solution to solid or from solid to solution

The chemical formula for gypsum is $CaSO_4 \cdot 2H_2O$ and the reversible reaction is as follows:

$$CaSO_4 \cdot 2H_2O \rightleftarrows C_a^{++} + SO_4^{=} + 2H_2O$$

Gypsum can be present in the solid phase or can be precipitated from a supersaturated solution. Gypsum is defined as a moderately soluble salt whose solubility product "Ksp" is equal to $2.4 \cdot 10^{-5}$. The solubility product is defined as follows:

$$Ksp = a_{Ca} \cdot a_{SO_4} \qquad (17)$$

where: a_{Ca} = activity of calcium ion

a_{SO_4} = activity of sulfate ion

From previous definitions

$$a_{Ca} = C_{Ca} \cdot \gamma_2$$

$$a_{SO_4} = C_{SO_4} \cdot \gamma_2$$

Substitution into equation (17)

$$Ksp = C_{Ca} \cdot \gamma_2 \cdot C_{SO_4} \cdot \gamma_2 \qquad (18)$$

To reiterate:

C_{Ca} = concentration of calcium ion in solution in units of moles per liter

C_{SO_4} = concentration of sulfate ion in solution in units of moles per liter

γ_2 = activity coefficient of divalent ion

$$\gamma_2 = \ell^{\frac{-4.68804 \cdot \sqrt{u}}{1 + \sqrt{u}}}$$

Let "X" = change in concentration in calcium and sulfate ions.

If: $X > 0$ - solution is undersaturated

$X = 0$ - solution is saturated

$X < 0$ - solution is supersaturated

Upon substitution equation (18) becomes:

$$Ksp = (C_{Ca} + X)\,(C_{SO_4} + X) \cdot \gamma_2^2$$

or:

$$0 = X^2 + (C_{Ca} + C_{SO_4})\,X - 2.4 \cdot 10^{-5}/\gamma_2^2$$

and:

$$X = \frac{-(C_{Ca} + C_{SO_4}) + \sqrt{(C_{Ca} + C_{SO_4})^2 - 4.0 \cdot \left(C_{Ca} \cdot C_{SO_4} - \dfrac{2.4 \cdot 10^{-5}}{\gamma_2^2}\right)}}{2.0}$$

Determination of change in concentration of ion pairs $CaSO_4^\circ$ and $MgSO_4^\circ$

Equation (3) defines the thermodynamic equilibrium constant - K_{CaSO_4} as follows:

$$K_{CaSO_4} = \frac{C_{Ca} \cdot \gamma_{Ca} \cdot C_{SO_4} \cdot \gamma_{SO_4}}{C_{CaSO_4}} = \frac{C_{Ca} \cdot C_{SO_4} \cdot \gamma_2^2}{C_{CaSO_4}} \qquad (19)$$

and: $K_{CaSO_4} = 4.9 \cdot 10^{-3}$ (experimentally derived)

Let: X = change of concentrations of calcium, sulfate, and calcium sulfate in solution in units of moles per liter. An increase in concentration in calcium and sulfate represents a decrease in the concentration of calcium sulfate then equation (19) can be expressed as follows with the inclusion of "X"

$$4.9 \cdot 10^{-3} = \frac{(C_{Ca} + X)\,(C_{SO_4} + X) \cdot \gamma_2^2}{(C_{CaSO_4} - X)}$$

or:

$$0 = (C_{Ca} + X)\,(C_{SO_4} + X) \cdot \gamma_2^2 - \left[\,4.9 \cdot 10^{-3}\,(C_{CaSO_4} - X)\,\right]$$

expanding:

$$0 = \gamma_2^2\,X^2 + \left[\,\gamma_2^2\,(C_{Ca} + C_{SO_4}) + 4.9 \cdot 10^{-3}\,\right] X + \gamma_2^2\,C_{Ca} \cdot C_{SO_4} - 4.9 \cdot 10^{-3}$$

Let:

$$a = \gamma_2^2$$

$$b = \gamma_2^2\,(C_{Ca} + C_{SO_4}) + 4.9 \cdot 10^{-3}$$

$$c = \gamma_2^2\,C_{Ca} \cdot C_{SO_4} - 4.9 \cdot 10^{-3}$$

and:

$$X = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

It is easily shown that the maximum concentration of $CaSO_4^\circ$ is a function of the two experimental constants Ksp and K_{CaSO_4} as follows:

$$Ksp = C_{Ca} \cdot C_{SO_4} \cdot \gamma_2^2$$

and:

$$K_{CaSO_4} = \frac{C_{Ca} \cdot C_{SO_4} \cdot \gamma_2^2}{C_{CaSO_4}}$$

then:

$$C_{CaSO_4}(\max) = \frac{Ksp}{K_{CaSO_4}} = \frac{2.4 \cdot 10^{-5}}{4.9 \cdot 10^{-3}} = 4.9 \cdot 10^{-3} \text{ moles per liter}$$

Equation (6) defines the thermodynamic equilibrium constant, K_{MgSO_4}, as follows:

$$K_{MgSO_4} = \frac{C_{Mg} \cdot \gamma_{Mg} \cdot C_{SO_4} \cdot \gamma_{SO_4}}{C_{MgSO_4}} = \frac{C_{Mg} \cdot C_{SO_4} \cdot \gamma_2^2}{C_{MgSO_4}} \qquad (20)$$

and: $K_{MgSO_4} = 5.9 \cdot 10^{-3}$ (experimentally derived)

Again let: X = change of concentration of magnesium, sulfate, and magnesium sulfate in solution in units of moles per liter. An increase in concentration in magnesium and sulfate represents a decrease in the concentration of magnesium sulfate.

Using the same algebra as was used for the change in $CaSO_4^{\circ}$, then:

$$0 = \gamma_2^2 X^2 + \left[\gamma_2^2 (C_{Mg} + C_{SO_4}) + 5.9 \cdot 10^{-3} \right] X + \gamma_2^2 C_{Mg} - 5.9 \cdot 10^{-3}$$

Let:

$$a = \gamma_2^2$$

$$b = \gamma_2^2 (C_{Mg} + C_{SO_4}) + 5.9 \cdot 10^{-3}$$

$$c = \gamma_2^2 C_{Mg} \cdot C_{SO_4} - 5.9 \cdot 10^{-3}$$

and

$$X = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

Determination of calcium-sodium exchange

Equation (13) defines the relationship of calcium and sodium ions as follows (Gapon):

$$N_{Na} = \frac{N_{Ca} \cdot C_{Na} \cdot \gamma_1}{K_2 \sqrt{C_{Ca}} \cdot \gamma_2}$$

Squaring both sides of the above equation

$$N_{Na}^2 = \frac{N_{Ca}^2 \cdot C_{Na}^2 \cdot \gamma_1^2}{K_2^2 \, C_{Ca} \cdot \gamma_2} \qquad (21)$$

Reiterating for terms in equation (21)

N_{Na} = concentration of sodium ion in solid phase (soil) in units of moles per gram

N_{Ca} = concentration of calcium ion in solid phase (soil) in units of moles per gram

C_{Na} = concentration of sodium ion in solution in units of moles per liter

C_{Ca} = concentration of calcium ion in solution in units of moles per liter

γ_1 and γ_2 = activity coefficients of monovalent and divalent ions, respectively

Let: X = change in concentration of calcium ion in the solid phase in units of moles per gram

then if X > 0:

Concentration of calcium ion in solid phase decreases

Concentration of calcium ion in solution increases

Concentration of sodium ion in solid phase increases

Concentration of sodium ion in solution decreases

and in terms of "X" then:

$$N_{Ca} = N_{Ca} - X$$

$$C_{Ca} = C_{Ca} + \beta X$$

$$N_{Na} = N_{Na} + 2X$$

$$C_{Na} = C_{Na} - \beta X$$

where:

β = conversion factor to convert moles per gram to moles per liter and must have units of grams per liter.

Substitution into equation (22):

$$(N_{Na} + 2X)^2 = \frac{(N_{Ca} - X)^2 \, (C_{Na} - 2\beta X)^2 \cdot \gamma_1^2}{K_2^2 \, (C_{Ca} + \beta X) \, \gamma_2}$$

and: $\gamma_2 = \gamma_1^4$

Let: $K_3 = 1/K_2 \ (Ca - Na)$

then:

$$\gamma_1^2 \, (N_{Na} + 2X)^2 \, (C_{Ca} + \beta X) = K_3^2 \, (N_{Ca} - X)^2 \, (C_{Na} - 2\beta X)^2$$

Expanding:

$$\gamma_1^2 N_{Na}^2 C_{Ca} + 4\gamma_1^2 N_{Na} C_{Ca} X + 4\gamma_1^2 C_{Ca} X^2 + \gamma^2 N^2_{Na} \beta X + 4\gamma_1^2 N_{Na} \beta X^2$$

$$+ 4\gamma_1^2 \beta X^3 - K_3^2 N_{Ca}^2 C_{Na}^2 + 2K_3^2 C_{Na}^2 N_{Ca} X - K_3^2 C_{Na}^2 X^2$$

$$+ 4K_3^2 N_{Ca}^2 C_{Na} \beta X - 8K_3^2 C_{Na} N_{Ca} \beta X^2 + 4K_3^2 C_{Na} \beta X^3 - 4K_3^2 N_{Ca}^2 \beta^2 X^2$$

$$+ 8K_3^2 N_{Ca} \beta^2 X^3 - 4K_3^2 \beta^2 X^4 = 0$$

Collecting terms:

X^4	X^3	X^2	X
$-4K_3^2 \beta^2$	$8K_3^2 N_{Ca} \beta^2$	$-4K_3^2 N_{Ca}^2 \beta^2$	$4K_3^2 N_{Ca}^2 C_{Na} \beta$
	$4K_3^2 C_{Na} \beta$	$-8K_3^2 C_{Na} N_{Ca} \beta$	$2K_3^2 C_{Na}^2 N_{Ca}$
	$4\gamma_1^2 \beta$	$-K_3^2 C_{Na}^2$	$4\gamma_1^2 N_{Na} C_{Ca}$
		$4\gamma_1^2 N_{Na} \beta$	$\gamma_1^2 N_{Na}^2 \beta$
		$4\gamma_1^2 C_{Ca}$	

K
$\gamma_1^2 N_{Na}^2 C_{Ca}$
$-K_3^2 N_{Ca}^2 C_{Na}^2$

The general equation for the above polynomial is:

$$AX^4 + BX^3 + CX^2 + DX + E$$

where:

$$A = -4K_s^2 \beta^2$$

$$B = 4\beta (2K_s^2 N_{Ca} + K_s^2 C_{Na} + \gamma_1^2)$$

$$C = 4\gamma_1^2 (N_{Na} \beta + C_{Ca}) - 4K_s^2 \beta N_{Ca} + 2C_{Na}) - K_s^2 C_{Na}^2$$

$$D = \gamma_1^2 N_{Na} (4C_{Ca} + \beta N_{Na}) + 2K_s^2 N_{Ca} C_{Na} (C_{Na} + 2\beta N_{Ca})$$

$$E = \gamma_1^2 N_{Na}^2 C_{Ca} - K_s^2 N_{Ca}^2 C_{Na}^2$$

Determination of Calcium-Magnesium Exchange

Equation (10) defines the relationship of calcium and magnesium as follows:

$$\frac{a_{Ca}}{a_{Mg}} = K_1 \frac{N_{Ca}}{N_{Mg}}$$

where:

a_{Ca} = the activity of the calcium ion in solution

a_{Mg} = the activity of the magnesium ion in solution

N_{Ca} = the concentration of the calcium ion in solid (soil) phase in units of moles per gram

N_{Mg} = the concentration of the magnesium ion in solid phase in units of moles per gram and:

$$a_{Ca} = C_{Ca} \cdot \gamma_2$$

$$a_{Mg} = C_{Mg} \cdot \gamma_2$$

where:

C_{Ca} = the concentration of the calcium ion in solution in units of moles per liter

C_{Mg} = the concentration of the magnesium ion in solution in units of moles per liter

γ_2 = activity coefficient of divalent ion

or:

$$\frac{C_{Ca} \cdot \gamma_2}{C_{Mg} \cdot \gamma_2} = K_1 \frac{N_{Ca}}{N_{Mg}} \qquad (22)$$

Let: X = change in concentration of ions in solid phase

and: $C_{Ca} = C_{Ca} + \beta X$

$C_{Mg} = C_{Mg} - \beta X$

$N_{Ca} = N_{Ca} - X$

$N_{Mg} = N_{Mg} + X$

Then if: $X > 0$

Concentration of calcium ion in solution increases

Concentration of calcium ion in solid decreases

Concentration of magnesium ion in solution decreases

Concentration of magnesium ion in solid increases

Substitution into equation (22)

$$\frac{(C_{Ca} + \beta X\,\gamma_2}{(C_{Mg} - \beta X)\gamma_2} = K_1\;\frac{N_{Ca} - X}{N_{Mg} + X}$$

or:

$$(C_{Ca} + \beta X)\,(N_{Mg} + X) = K_1\,(C_{Mg} - \beta X)\,(N_{Ca} - X)$$

expanding:

$$C_{Ca}\,N_{Mg} + (C_{Ca} + \beta N_{Mg})\,X + \beta X^2 = K_1\left[\,C_{Mg}\,N_{Ca} - (C_{Mg} + \beta N_{Ca})\,X + \beta X^2\,\right]$$

Collecting terms:

$$\beta\,(1 - K_1)\,X^2 + \left[\,\beta\,(N_{Mg} + K_1 N_{Ca}) + K_1\,C_{Mg} + C_{Ca}\,\right] X - K_1 C_{Mg} N_{Ca}$$

$$+ C_{Ca} N_{Mg} = 0.$$

Let: $A = \beta\,(1 - K_1)$

$B = \beta\,(N_{Mg} + K_1 N_{Ca}) + K_1 C_{Mg} + C_{Ca}$

$C = C_{Ca} N_{Mg} - K_1 C_{Mg} N_{Ca}$

or:

$$X = \frac{-B + \sqrt{B^2 - 4AC}}{2A}$$

COMPUTER PROGRAM LISTING FOR SIMULATION MODELING

```
      PROGRAM ACUMEN
C**** THIS COMPUTER APPLICATION HAS BEEN DESIGNED AS A SYSTEM ANALYSIS
C**** AND CONJUNCTIVE USE MODEL EMULATING A NODAL CONCEPT IN DIVIDING
C**** A WATER BASIN INTO PERTINENT FUNCTIONAL OR RESPONSIVE CRITICAL
C**** AREAS ALLOWING AS MUCH FLEXIBILITY IN MODEL DESIGN AS WAS
C**** CONSIDERED PRACTICAL
      COMMON / GENRL / LTITLE(8), NCTRL(20, 3), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMNOD, ISEQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
      COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     PDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,8)
      COMMON / PROPER / SOIL(20, 10, 21), RTANK(20, 10), TTANK(20, 10),
     1 GRTANK(20, 10)  , NSEG (20) , CONUSE (20, 10, 30)
     2              , KUSE (20, 10, 30)
      COMMON / POWER / CAPBAB(20, 20), TDATA(20, 4), ENERGY(20, 8), PDA
     ATA(20, 12)
      COMMON / SALT / QTOT(20, 20), WQAL(20, 20)
      COMMON / PARAM / REGRES ( 20, 11 ) , REGWR ( 20, 10 ) ,
     1        PREDIC ( 20, 10 ) , OBSVAL (20,10), CHEMDM ( 20, 10, 10)
      DIMENSION  QINRIV (10), NPASS (20), CRSERV (10), KFA (20) ,
     1           QFLOW (10 ) , TEMP (10)
      EQUIVALENCE ( CONUSE, KUSE )
      DATA ( IFIR = 0 )
      IF ( IFIR . NE. 0 )  GO TO 10
C**** THIS IS THE FIRST TIME PROGRAM HAS BEEN ENTERED FOR A PARTICULAR
C**** JOB - SET READ AND WRITE UNITS AND READ SYSTEM STRUCTURE AND
C**** PERTINENT INITIALIZATION PARAMETERS
      IR = 60
      IW = 61
      LINE = 0
      DO 5 K = 1, 4
      JREAD = K
      CALL PERUSE ( JREAD , IW , IR )
    5 CONTINUE
      IFIR = 1
      MO = MOBEG
      IYR = IYRBEG
C**** INITIAILIZE PASS INDEX OF EACH NODE FOR USE IN ITERATIVE SCHEME
   10 DO 15 K = 1, 20
      NPASS ( K ) = 0
   15 CONTINUE
C**** INITIALIZE STARTING INDICES FOR NODE (MIN) AND SEQUENCE ( MINA )
C**** LOOPS
      MIN = 1
      MINA = 1
      WRITE ( IW , 16 )
   16 FORMAT ( 1H1, 8X )
C**** BEGIN ITERATIVE SCHEME FOR EACH NODE WHERE NUMNOD = NUMBER OF NODES
   20 DO 600 KN = MIN , NUMNOD
C**** CHECK TO DETERMINE IF THIS IS THE FIRST PASS THROUGH THIS NODE
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      PROGRAM ACUMEN
C**** THIS IS THE FIRST PASS THROUGH THIS NODE ** INITIALIZE RIVER
C**** FLOW AND CHEMISTRY ARRAY ( QINRIV ) AND UPDATE AQUIFER ASSUME ONE
C**** MONTH LAG IN CHEMISTRY MIX ** LET ARRAY BEGWR = BEGINNING
C**** CONDITIONS OF AQUIFER AT START OF TIME FRAME
      DO 25 K = 1, 10
      QINRIV (K) = 0.0
      BTANK ( KN, K ) = 0.0
      TTANK ( KN, K ) = 0.0
      BEGWR (KN, K ) = GRTANK ( KN, K )
   25 CONTINUE
C**** THIS PORTION OF THE SUBROUTINE IS USED FOR ALL PASSES ** LET NS=
C**** NUMBER OF SEQUENTIAL OPERATIONS IN THIS NODE
   30 NS = NUMSEQ ( KN)
C**** LOOP THROUGH EACH SEQUENCE IN NODE
      DO 500 KS = MINA , NS
      IS = IABS ( ISEQ (KN, KS ) )
      IF ( ISEQ (KN, KS)) 50, 350, 400
   50 CONST = DEMAND ( KN, IS, MO )
      TEST = DEMAND ( KN, IS, 14)
      IF ( TEST .GT. 2.0. AND. TEST . LT. 6.0 ) GO TO 250
C**** THIS OPERATIONAL SEQUENCE REPRESENTS A DEMAND IN THE NODE
C**** WHOSE SOURCE MAY BE FROM THE RIVER ( SURFACE FLOW ) OR FROM THE
C**** AQUIFER ( SUBSURFACE FLOW ) TO SUPPLY EITHER AN IRRIGATION
C**** OR A MUNICIPAL AND INDUSTRIAL REQUIREMENT
      IF ( DEMAND (KN, IS, 13 ) .GT. 1.0 )  GO TO 170
C**** DEMAND IS TO BE SUPPLIED FROM RIVER ( SURFACE FLOW)
      IF ( TEST . EQ. 6.0 ) GO TO 230
      TEMPR = QINRIV (1) - CONST
      IF ( ABS (TEMPR).LT. 1.0 )  TEMPP = 0.0
      IF ( TEMPR . LT. 0.0 ) GO TO 90
C**** DEMAND CAN BE FULLY MET BY FLOW IN THE RIVER SET INDEX (INDY) = 1
      INDY = 1
C**** CALL RETURN FLOW AND SHORTAGE SUBROUTINE ( RFCOMP ) TO COMPUTE
C**** AND ALLOCATE RETURN FLOW MAGNITUDE AND CHEMISTRY AND COMPARE
C**** SHORTAGE ( IF ANY ) WITH SHORTAGE INDEX ** IF THE TEST FAILS THE
C**** SHORTAGE CRITERIA RFCOMP WILL TERMINATE COMPUTATION
   60 CALL RFCOMP ( QINRIV, KN, IS, INDY, MO, CONST, IW )
C**** SET ACTUAL DIVERSION AND CHEMISTRY OF WATERS DIVERTED
   70 DEMAND ( KN, IS, 16 ) = CONST
      QINRIV (1) = TEMPR
      DO 80 K = 2, 10
      CHEMDM ( KN, IS , K ) = QINRIV (K)
   80 CONTINUE
      GO TO 500
C**** DEMAND CAN NOT BE FULLY SUPPLIED BY FLOW IN THE RIVER SEARCH
C**** UPSTREAM RESERVOIRS FOR POSSIBLE RELEASES - MAKE RELEASES FROM
C**** RESERVOIRS ON THE BASIS OF AN IDEAL RANKING PROCESS.
   90 CALL DTABLE ( KN, KFA, IC, KS )
C**** CHECK TO DETERMINE IF RESERVOIRS EXIST ABOVE DEMAND POINT
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      PROGRAM ACUMEN

C**** THERE ARE NO UPSTREAM RESERVOIRS AVAILABLE FOR ADDITIONAL RELEASES
C**** SET DIVERSION EQUAL TO FLOW IN RIVER AND CALL ROUTINE RECOMP
C**** TO DETERMINE IF SHORTAGE IS TOLERABLE AND COMPUTE RETURN FLOW
C**** AND ALLOCATION. IF SHORTAGE IS NOT TOLERABLE ROUTINE RECOMP WILL
C**** TERMINATE COMPUTATION
  100 INDY = 2
      CONST = QINRIV (1)
      TEMPR = 0.0
      GO TO 60
C**** SEARCH FOR AVAILABLE UPSTREAM RESERVOIRS FOR POSSIBLE ADDITIONAL
C**** RELEASES TO MEET THIS DEFICIT
  110 DO 140 K = 1, IC
      KFAK = KFA (K)
      KNODE = NFIND ( KFAK )
C**** CHECK TO DETERMINE IF THIS RESERVOIR IS CONSTRAINED IN MAKING
C**** ADDITIONAL RELEASES
      IF ( NPASS ( KNODE ) . EQ. 100 )  GO TO 140
C**** LET PRELM = TOTAL RELEASE MADE DURING PREVIOUS PASS OR CALL
      PRELM = RDATA ( KNODE ,10 )
C**** TEMPR = RELEASE REQUIRED TO MEET DEFICIT
      QFLOW (1) = TEMPR
      CALL RESOPR ( QFLOW , KN, MO, IW )
C**** LET DELTAF = ADDITIONAL RELEASE  (IF ANY )
      DELTAF = RDATA ( KNODE , 10 ) - PRELM
      IF ( DELTAF . GT. 0.0 ) GO TO 120
      NPASS ( KNODE ) = 100
      GO TO 140
C**** ADDITIONAL RELEASE CAN BE MADE ** SET LOOP INDICES FOR RE-ENTRY
C**** INTO ITERATIVE SCHEME
  120 TEMPR = TEMPR + DELTAF
      NPASS ( KNODE ) = 1
      IF ( TEMPR . LT. 0.0 ) NPASS ( KNODE ) = 100
C**** UPDATE VOLUME AND CHEMISTRY OF RIVER FLOW BELOW RESERVOIR
      DO 125 KA = 2, 10
      QINRIV ( KA ) = QFLOW (KA)
  125 CONTINUE
      QINRIV (1) = RDATA ( KNODE , 10 )
C**** RESET LOOP INDICES
      NS = NUMSEQ (KNODE )
      DO 130 KA = 1, NS
      KX = KA
      IF ( ISEQ ( KNODE , KA ) . EQ. 0 ) GO TO 135
  130 CONTINUE
      GO TO 1040
C**** NOTE **** A RESERVOIR CANNOT BE THE LAST SEQUENCE OF OPERATIONS
C**** IN A NODE ****
  135 IF ( KX . EQ. NS )   GO TO 1050
      MIN = KNODE
      MINA = KX + 1
  140 CONTINUE
C**** ALL RESERVOIRS HAVE BEEN SEARCHED AND NO ADDITIONAL RELEASES CAN
C**** BE MADE TO MEET DEFICIT
      GO TO 100
C**** DEMAND IS TO BE SUPPLIED FROM AQUIFER ( SUBSURFACE FLOW )
  170 TEMPR = GRTANK ( KN, 1 ) - CONST
      IF ( TEST .EQ. 6.0 )  GO TO 340
      IF ( ABS ( TEMPR ) .LT. 1.0 ) TEMPR = 0.0
      IF ( TEMPR . LT. 0.0 ) GO TO 220
C**** DEMAND CAN BE FULLY SUPPLIED FROM AQUIFER ( SUBSURFACE FLOW )
C**** SET INDEX (INDY) = 1
      INDY = 1
C**** CALL RETURN FLOW AND SHORTAGE SUBROUTINE ( RFCOMP ) TO COMPUTE
C**** AND ALLOCATE RETURN FLOW MAGNITUDE AND CHEMISTRY AND COMPARE
C**** SHORTAGE ( IF ANY ) WITH SHORTAGE INDEX ** IF THE TEST FAILS THE
C**** SHORTAGE CRITERIA RFCOMP WILL TERMINATE COMPUTATION
  180 DO 185 K = 2, 10
      TEMP (K) = BEGWR ( KN, K )
  185 CONTINUE
      CALL RFCOMP ( TEMP  , KN, IS, INDY, MO, CONST, IW )
      GRTANK ( KN, 1 ) = TEMPR
C**** SET ACTUAL DIVERSION AND CHEMISTRY OF WATERS DIVERTED
  190 DEMAND ( KN , IS, 16 ) = CONST
      DO 200 K = 2, 10
      CHEMDM ( KN, IS, K ) = BEGWR ( KN, K )
  200 CONTINUE
      GO TO 500
C**** DEMAND CAN NOT BE FULLY SUPPLIED BY AQUIFER- COMPUTE SHORTAGE
C**** RETURN FLOW AND ALLOCATION ( IF SHORTAGE NOT TOLERABLE RFCOMP
C**** WILL TERMINATE COMPUTATION )
  220 CONST = GRTANK ( KN, 1 )
      INDY = 2
      TEMPR = 0.0
      GO TO 190
C**** THIS DEMAND REPRESENTS A SURFACE FLOW THAT IS TRANSFERRED OUT
C**** OF SYSTEM
  230 TEMPR = QINRIV (1) - CONST
      IF ( TEMPR . LT. 0.0 )   GO TO 1010
      GO TO 70
C**** WHEN DEMAND ( KN, IS, 14) THE DESTINATION OR USE INDEX IS GREATER
C**** THAN 2.0 SIMPLE TRANSFERS OF FLOW ARE TREATED AS DEMANDS SO THAT
C**** ROUTINE RFCOMP WILL SET UP THE PROPER QINFLO ARRAY. THESE TRANSFERS
C**** CAN HAVE PERCOMPUTED VOLUMES (INPUT DATA ) OR WILL BE COMPUTED IN
C**** SIMULATION
  250 IF ( DEMAND ( KN, IS, 13 ) .GT. 1.0 ) GO TO 290
C**** TRANSFERS WILL BE MADE FROM THE RIVER (SURFACE FLOW) TO AQUIFER
C**** OR SOIL COLUMN
      IF ( TEST.EQ. 3 )   INDY = 3
      IF ( TEST.EQ. 4 )   INDY = 4
      IF ( ABS (TFMPR) .LT. 1.0 )  TEMPR = 0.0
      IF ( TEMPR . LT. 0.0 )  GO TO 1060
      GO TO 60
C**** TRANSFERS WILL BE MADE FROM THE AQUIFER (SUBSURFACE FLOW ) TO THE
C**** RIVER ** CONDITIONALLY IF THE AQUIFER IN ANY NODE CANNOT MEET THE
C**** TRANSFER REQUIREMENT.  AN INTERNODAL TRANSFER TO THE RIVER WILL
C**** BE ALLOWED ONLY FROM THE NODE IMMEDIATELY UPSTREAM OF THE NODE
C**** IN DEFICIT
  290 TEMPR =  GRTANK ( KN, 1 ) - CONST
      IF ( ABS ( TEMPR ) . LT. 1.0 )  TEMPR = 0.0
      IF ( KN. GT. 1 )  GO TO 295
      IF ( TEMPR . LT. 0.0 )  GO TO 1070
      GO TO 180
C**** SET QINFLO ARRAY ** LET NODE = KUSE ( KN, IS, 24) AND SEQUENCE =
C**** KU[illegible] ( KN, IS , 25 ) .  ALSO SET UPSTREAM AQUIFER NODE = KUSE
C**** [illegible], IS, 2P ) FOR INTERNODAL TRANSFER ( IF REQUIRED )
  295 [illegible] = KUSE ( KN, IS, 28 )
      IF ( LN . EQ. 0 )  GO TO 1070
      KG = NFIND ( LN )
      LN = KUSE ( KN, IS, 24 )
      IF ( LN . EQ. 0 )  GO TO 1070
      KP = NFIND ( LN )
      KZ = KUSE ( KN, IS , 25 )
      IF ( TEMPR . LT. 0.0 )  GO TO 310
C**** NO INTERNODAL TRANSFER REQUIRED
      DO 300 K = 1, 10
      QINFLO ( KP, KZ, K ) = 0.0
  300 CONTINUE
      GO TO 180
C**** AN INTERNODAL TRANSFER IS REQUIRED CHECK CONDITIONS OF AQUIFER IN
C**** UPSTREAM NODE
  310 COMP = ABS ( TEMPR )
      COMPA = GRTANK ( KG, 1 ) - COMP
      IF ( COMPA . LT. 0.0 )  GO TO 1070
C**** UPSTREAM AQUIFER CAN MEET DEFICIT SET QINFLO AND GRTANK ARRAYS
      GRTANK ( KG, 1 ) = COMPA
      DO 320 K = 2, 10
      QINFLO ( KP, KZ, K ) = GRTANK ( KG , K )
  320 CONTINUE
      QINFLO ( KP, KZ, 1 ) = COMP
      TEMPR = 0.0
      GO TO 180
C**** THIS DEMAND REPRESENTS A SUBSURFACE FLOW THAT IS TRANSFERRED
C**** OUT OF SYSTFM
  340 IF ( TEMPR . LT. 0.0 )  GO TO 1020
      GO TO 190
C**** THIS IS A RFSERVOIR UPDATE
  350 CALL RESOPR ( QINRIV , KN , MO , IW )
      MODE = 1
      PROGRAM ACUMEN

C**** THIS PORTION OF THE PROGRAM INCLUDES THE VOLUME AND CHEMISTRY
C**** UPDATES FOR ALL INFLOWS TO THE NODE
  400 DO 410 K = 1, 10
      TEMP (K) = QINFLO ( KN, IS, K )
  410 CONTINUE
      TEST = QINFLO (KN, IS, 11 )
      CONST = QINFLO (KN, IS, 1 )
      IF ( TEST . NE. 1.0 )  GO TO 430
C**** THIS IS AN INFLOW TO THE RIVER
      CALL CHEMRV ( QINRIV, CONST, KN, IS )
      QINRIV(1) = QINRIV (1) + CONST
      GO TO 500
  430 IF ( TEST . NE. 2.0 )  GO TO 440
C**** THIS IS AN INFLOW TO THE AQUIFER
      CALL CHEMGR ( TEMP, CONST, KN, IS )
      GRTANK ( KN, 1) = GRTANK (KN, 1 ) + CONST
      GO TO 500
  440 IF ( TEST . NE. 3.0 )  GO TO 450
C**** THIS IS AN INFLOW TO THE PONDING POOL
      CALL CHEMTT ( TEMP, CONST, KN, IS )
      TTANK ( KN, 1 ) = TTANK ( KN, 1 ) + CONST
      GO TO 500
  450 IF ( TEST .NE. 4.0 )  GO TO 1000
C**** AT THIS POINT IN THE MODEL CRITERIA FOR THE OPERATION OF THE
C**** SYSTEM IS REQUIRED.  THE OPERATIONAL CRITERIA SHOULD BE FORMULATED
C**** AND INSERTED AS A SUBROUTINE OR A SERIES OF SUBROUTINES AND/OR
C**** FUNCTIONS WHICH ARE MONITORED BY THE SUBROUTINE CALLED AT THIS
C**** POINT.  THE TECHNIQUE AS OUTLINED DOES NOT DESTROY THE
C**** GENERALIZED CONCEPT OF THE MODEL.
C**** THIS AN OBSERVED CHECK POINT
C**** CALL VERNAL SUBROUTINE TO SIMULATE TRANSFERS OF FLOW
C**** BETWEEN SURFACE AND SUBSURFACE FACILITIES TO OBTAIN HYDRAULIC
C**** BALANCE IN NODE
      CALL VERNAL ( KN, IS, MO, OBSERV, QINRIV )
  500 CONTINUE
C**** CHECK TO DETERMINE IF A SOIL COLUMN EXISTS IN THIS NODE
      IF ( TTANK ( KN, 1 ) . LE. 0.0 ) GO TO 540
C**** CHECK TO DETERMINE IF SOIL COLUMN DATA EXISTS FOR THIS NODE
      NSOIL = NSEG (KN )
      IF ( NSOIL . EQ. 0 ) GO TO 1030
C**** SOIL COLUMN DATA EXISTS PERCOLATE WATERS IN TTANK THROUGH
C**** SOIL COLUMN INTO BTANK
      CALL SOILCO ( KN, IW, IR, NSOIL )
C**** UPDATE AQUIFER WITH LINEAR MIX WITH WATER IN BTANK
      BTANK (KN, 1) = TTANK ( KN, 1 )
      DO 520 K = 1, 10
      TEMP (K) = BTANK ( KN, K )
  520 CONTINUE
      CALL CONVER ( TEMP , 2 )
      PROGRAM ACUMEN

C**** SET UP TRANSFERS OF OUTFLOW FROM THIS NODE TO NEXT LOWER
C**** NODE - WHERF ND= NODE NUMBFR OF NEXT LOWER NODE AND NS =
C**** ENTERING SEQUFNCE OF NEXT LOWER NODE
  540 ND = NCTRL ( KN, 2 )
      IF ( KN . EQ. NUMNOD )  GO TO 560
      ND = NFIND (ND)
      NS = NCTRL ( KN, 3 )
      DO 550 K = 1, 10
      QINFLO (ND, NS, K) = OBSERV (K)
  550 CONTINUE
  560 DO 570 K = 1, 10
      PREDIC ( KN, K ) = QINRIV (K)
      OBSVAL ( KN, K ) = OBSERV (K)
  570 CONTINUE
  600 CONTINUE
      CALL WRIT ( MO, IYR, IW )
      MC = MO + 1
      IF ( MO . LE. 12 ) GO TO 750
      MO = 1
      IYR = IYR + 1
  750 IF ( IYR . LT. IYREND )  GO TO 770
      IF ( MO . GT. MOEND )  CALL EXIT
  770 JREAD = 5
      CALL PERUSE ( JREAD , IW, IR )
      GO TO 10
C**** PROGRAM CONTROLLED ERROR MESSAGES ARE GENERATED HFRE
 1000 WRITE ( IW, 1005 ) TEST
 1005 FORMAT ( 1H1, 7X, 20HDESTINATION INDEX = ,F3.0,12H IS IN ERROR )
      GO TO 1500
 1010 WRITE ( IW, 1015)
 1015 FORMAT(1H1,7X,45HDEMAND LEAVING SYSTEM FROM SURFACE IN DEFICIT)
      GO TO 1500
 1020 WRITE ( IW, 1025 )
 1025 FORMAT(1H1,7X,48HDEMAND LEAVING SYSTEM FROM SUBSURFACE IN DEFICIT)
      GO TO 1500
 1030 WRITE ( IW , 1035 )
 1035 FORMAT ( 1H1, 7X, 25HNO SOIL COLUMN DATA FOUND    )
      GO TO 1500
 1040 WRITE ( IW , 1045 )
 1045 FORMAT(1H1,7X,46HNO RESERVOIR FOUND IN SEARCH OF SEQUENCE ARRAY )
      GO TO 1500
 1050 WRITE ( IW , 1055 )
 1055 FORMAT ( 1H1, 7X, 39HRESERVOIR IS LAST OPERATION IN SEQUENCE  )
      GO TO 1500
 1060 WRITE ( IW , 1065 )
 1065 FORMAT ( 1H1, 7X, 42HSURFACE TRANSFER AS A DEMAND IS IN DEFICIT )
      GO TO 1500
 1070 WRITE ( IW , 1075 )
 1075 FORMAT ( 1H1, 7X,45HSUBSURFACE TRANSFER AS A DEMAND IS IN DEFICIT)
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      PROGRAM ACUMEN

 1500 WRITE ( IW, 1510 ) KN , IS
 1510 FORMAT ( 8X, 12HFOR NODE =    , I3, 8X, 10HSEQ.NO. =  , I3 )
      CALL EXIT
      END
      SUBROUTINE PERUSE (JREAD , IW, IR )

       COMMON / GENRL / LTITLE(8), NCTRL(20, 3), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMMOD, ISEQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
       COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     BDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAGUNM (20,8)
       COMMON / POWER / CAPBAB(20, 20), TDATA(20, 4), ENERGY(20, 8), PDA
     ATA(20, 12)
       COMMON / PROPER / SOIL(20, 10, 21), BTANK(20, 10), TTANK(20, 10),
     1 GRTANK(20, 10)  , NSEG (20) , CONUSE (20, 10, 30)
     2            , KUSE (20, 10, 30)
      EQUIVALENCE ( CONUSE, KUSE )
       DIMENSION LTEMP(22), CTEMP(15)
C**** SET READ AND WRITE LOGICAL UNITS
C**** WRITE INPUT LISTING HEADING AND VALUES OF JREAD
      WRITE ( IW, 10 )
   10 FORMAT  (1H1, 24X, 33H ***  LISTING OF INPUT DATA  ***  / / )
      WRITE ( IW , 30 ) JREAD
   30 FORMAT  (1H , 8HJREAD = , I3 )
C
C***** WHEN JREAD = 1 READ AND STORE SYSTEM STRUCTURE - CONCLUDE THIS
C*****READ WITH CARD CONTAINING THE WORD CONEND IN THE FIRST SIX COLUMNS
C
C*****WHEN JREAD = 2 READ AND STORE TITLES AND INITIAL CONDITIONS OF
C*****SURFACE RESERVOIRS AND AQUIFERS ( SUBSURFACE RESERVOIRS).
C*****ALSO  WHEN JREAD = 2 READ AND STORE INITIAL SOIL CONTITIONS AS
C*****WELL AS SOIL COLUMN PHYSICAL FEATURES. CONCLUDE THIS READ WITH
C*****CARD CONTAINING THE WORD COLEND IN THE FIRST SIX COLUMNS
C
C*****WHEN JREAD = 3 READ AND STORE MATHEMATICAL REPRESENTATIONS OF
C*****PERTINENT SURFACE FACILITIES PHYSICAL FEATURES . CONCLUDE THIS
C*****READ WITH CARD CONTAINING EQUEND IN THE FIRST SIX COLUMNS
C
C*****WHEN JREAD = 4 READ INFLOWS AND DEMANDS WITH TITLES FOR THE FIRST TI
C*****FRAME ONLY NOTE ** TITLE MUST PRECEDE EACH INFLOW AND DEMAND DATA
C*****CONCLUDE THIS READ WITH CARD CONTAINING THE WORD ENDATA IN THE
C*****FIRST SIX COLUMNS
C
C*****WHEN JREAD = 5 READ INFLOW AND DEMAND DATA CARDS SUSEQUENT TO THE
C*****FIRST TIME FRAME AS WELL AS ANY TRANSACTION CARDS-- CONCLUDE THIS
C*****READ WITH CARD CONTAINING THE WORD ENDATA IN THE FIRST SIX COLUMNS
      GO TO ( 40, 220, 450, 600, 650 ) , JREAD
C**** READ SYSTEM CONTROL CARDS
   40 READ ( IR, 60 ) LTITLE, KPRI
   60 FORMAT  (8A8, I16)
      WRITE ( IW, 80 ) LTITLE , KPRI
   80 FORMAT  (1H , 8A8, I16)
      JK= 0
      JJ = 0
  100 READ ( IR, 120 ) IONE , ITWO , LTEMP
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      SUBROUTINE REPUSE (JREAD , IW, IR )

      WRITE ( IW, 140 ) IONE , ITWO , LTEMP
  140 FORMAT  (1H , 2R3,22I3)
C**** STORE SYSTEM CONTROL DATA
      IF ( IONE . NE. 3RCON )   GO TO 1000
      IF ( ITWO . NE. 3RNOD )  GO TO 160
      JK = JK + 1
      NUMNOD = JK
      DO 150 K = 1, 3
      NCTRL (JK, K ) = LTEMP (K)
  150 CONTINUE
      GO TO 100
  160 IF ( ITWO . NE. 3RSEQ ) GO TO 190
      JK = NFIND ( LTEMP (1) )
C**** STORE NUMBER OF SEQUENCE POINTS IN A NODE
      NUMSEQ (JK) = LTEMP (2)
      NS = LTEMP (2)
C**** CHECK TO DETERMINE IF NUMBER OF SEQUENCE POINTS EXCEED 20
      IF ( NS . GT. 20 )  GO TO 1020
      DO 170 K = 1, NS
      KX = K + 2
      ISEQ (JK, K ) = LTEMP (KX)
  170 CONTINUE
      GO TO 100
  190 IF ( ITWO . NE. 3RWAT )  GO TO 210
      JK = NFIND ( LTEMP (1) )
C**** STORE SYSTEM FLOW ARRAY
      DO 200 K = 1, 20
      KX = K + 2
      NDWTR ( JK, K ) = LTEMP (KX)
  200 CONTINUE
      GO TO 100
  210 IF ( ITWO . NE. 3REND )  GO TO 1040
C**** STORE DATES FOR BEGINNING AND END OF STUDY PERIOD
      MOBEG = LTEMP (1)
      IYRBEG = LTEMP (2)
      MOEND = LTEMP (3)
      IYREND = LTEMP (4)
      GO TO 2000
C**** READ AND STORE INITIAL VALUES AND MATHEMATICAL REPRESENTATIONS
C**** OF SYSTEM PHYSICAL FEATURES AS WELL AS TITLES OF SAME IF
C**** APPLICABLE - SOIL COLUMN INITIAL AND PHYSICAL DATA ARE INCLUDED
C**** IN THIS PORTION OF THE SUBROUTINE
  220 READ  (IR, 230) IONE, ITWO, (LTEMP(I), I = 1, 11)
  230 FORMAT  (2R3,I2, 1X, I3, R3, 8A8)
      WRITE  (IW, 240) IONE, ITWO, (LTEMP(I), I = 1, 11)
  240 FORMAT  (1H , 2R3,I2, 1X, I3, R3, 8A8)
      IF ( IONE . NE. 3RAQU ) GO TO 260
C**** STORE TITLE OF AQUIFER ( SUBSURFACE RESERVOIR )
      JK = NFIND ( LTEMP (2) )
      SUBROUTINE PERUSE (JREAD , IW, IR )

      KX = K + 3
      KAQUNM ( JK, K ) = LTEMP ( KX )
  250 CONTINUE
      GO TO 280
  260 IF ( IONE . NE. 3RSUR )   GO TO 370
C**** STORE TITLE OF SURFACE RESERVOIR
      JK = NFIND ( LTEMP (2) )
      DO 270 K = 1, 8
      KSURNM ( JK, K ) = LTEMP (KX)
  270 CONTINUE
  280 READ  (IR, 290) IONE, ITWO, (LTEMP(I), I = 1, 4), (CTEMP(J), J = 1
     A, 10), (LTEMP(K), K = 5, 7)
  290 FORMAT  (2R3,I2, I1, I3, R3, 10F6.0, I2, I1, I2)
      WRITE  (IW, 300) IONE, ITWO, (LTEMP(I), I = 1, 4), (CTEMP(J), J =
     A1, 10), (LTEMP(K), K = 5, 7)
  300 FORMAT  (1H , 2R3,I2, I1, I3, R3, 10F6.0, I2, I1, I2)
      IF ( IONE . NE. 3RRES ) GO TO 340
C**** STORE DATA FOR SURFACE RESERVOIR IN RDATA ARRAY
      JK = NFIND ( LTEMP (3))
C**** LET NEXP REPRESENT POWER OF 10 USED IN REPORTING FLOW MAGNITUDES
      NEXP = LTEMP (6)
      FAC = 10.0 ** NEXP
      RDATA (JK, 1 ) = LTEMP (3)
      RDATA (JK, 2 ) = LTEMP (1)
      RDATA ( JK, 3) = CTEMP (1) * FAC
      DO 310 K = 2, 5
      KA = K + 9
      RDATA ( JK, KA ) = CTEMP (K) * FAC
  310 CONTINUE
      RDATA ( JK, 20 ) = CTEMP (6) * FAC
C**** CARD CONTAINING RESERVOIR CHEMISTRY DATA MUST ALWAYS FOLLOW
C**** PHYSICAL DATA CARD - UNITS OF CONCENTRATION CAN BE IN MEQ/ LITER
C**** OR PARTS PER MILLION LTEMP (2) CONTAINS THIS UNITS INDEX
      READ  (IR, 290) IONE, ITWO, (LTEMP(I), I = 1, 4), (CTEMP(J), J = 1
     A, 10), (LTEMP(K), K = 5, 7)
      IF ( ITWO .NE. 3RCHM )  GO TO 1060
      WRITE  (IW, 300) IONE, ITWO, (LTEMP(I), I = 1, 4), (CTEMP(J), J =
     A1, 10), (LTEMP(K), K = 5, 7)
      JK = NFIND (LTEMP (3 ))
C**** CHECK TO DETERMINE IF ONLY TOTAL SALTS IN PPM ARE REPORTED
      IF ( CTEMP (10) . GT. 0.0 ) GO TO 320
C**** CONCENTRATIONS OF CONSTITUENTS ARE REPORTED CONVERT TO PPM
C**** AND COMPUTE TOTAL SALTS ON BASIS OF CONCENTRATIONS
      CALL CONVER ( CTEMP , LTEMP (2))
  320 DO 330 K = 2, 10
      KX = K + 99
      RDATA (JK, KX ) = CTEMP (K)
  330 CONTINUE
      GO TO 220
      SUBROUTINE PERUSE (JREAD , IW, IR )

C**** STORE INITIAL CAPACITY AND CHEMISTRY FOR AQUIFER
      JK = NFIND ( LTEMP(3))
C**** CHECK TO DETERMINE IF ONLY TOTAL SALTS IN PPM ARE REPORTED
      IF(CTEMP (10) . GT. 0.0 )  GO TO 350
C**** CONCENTRATIONS OF CONSTITUENTS ARE REPORTED CONVERT TO PPM
C**** AND COMPUTE TOTAL SALTS ON BASIS OF CONCENTRATIONS
      CALL CONVER ( CTEMP, LTEMP (2) )
  350 DO 360 K = 2, 10
      GRTANK ( JK, K ) = CTEMP (K)
  360 CONTINUE
      NEXP = LTEMP (6)
      FAC = 10.0 ** NEXP
      GRTANK ( JK, 1 ) = CTEMP (1) * FAC
      GO TO 220
C**** READ SOIL DATA FOR SOIL COLUMN - EACH SEGMENT IN SOIL COLUMN MUST
C**** BE IN PROPER SEQUENCE.  SEGMENT NUMBER ONE IS SEGMENT NEAREST
C**** GROUND SURFACE.
  370 IF ( IONE . NE. 3RCOL  ) GO TO 1080
      IF ( ITWO .EQ. 3REND )    GO TO 2000
      IF ( ITWO . NE. 3RSEG  ) GO TO 1100
      LSEG = 0
      KNODE = LTEMP(2)
      JK = NFIND (KNODE )
      NSEG ( JK) = LTEMP (1)
      LNODE = KNODE
      MAX = NSEG (JK)
      DO 400 J = 1, MAX
      READ(IR,380) IONE,ITWO, (LTEMP (KA), KA=1,2), (CTEMP(KB),KB=1,15)
  380 FORMAT(2R3,2I3,8F5.0,F3.0,3F5.0, F1.0, F4.0,F5.0)
      WRITE(IW,390)IONE,ITWO, (LTEMP (KA), KA=1,2), (CTEMP(KB),KB=1,15)
  390 FORMAT(1H ,2R3, 2I3, 8F5.0, F3.0, 3F5.0, F1.0, F4.0, F5.0 )
      IF ( IONE .NE. 3RCOL )    GO TO 1100
      IF ( ITWO .NE. 3RSEG  )    GO TO 1100
      KNODE = LTEMP (1)
      IF ( KNODE . NE. LNODE  ) GO TO 1100
      LSEG = LSEG + 1
      IF ( LSEG .NE. LTEMP (2)) GO TO 1100
      KS = LSEG
      DO 400 K = 1, 15
      SOIL ( JK, KS, K ) = CTEMP (K)
  400 CONTINUE
      GO TO 220
C**** READ AND STORE MATHEMATICAL REPRESENTATIONS OF PHYSICAL FEATURES
C**** OF SURFACE FACILITIES
  450 READ ( IR, 460 ) IONE , ITWO , KNOD , (LTEMP (K) , CTEMP (K) ,
     1          K= 1, 4 ) , CTEMP (5)
  460 FORMAT ( 2R3, I4, 4 ( I3, F12.0 ) , F10.0 )
      WRITE ( IW, 465 ) IONE, ITWO, KNOD , ( LTEMP (K) , CTEMP(K) ,
     1                    K = 1,4 ), CTEMP (5)
```

```
      SUBROUTINE PERUSE (JREAD , IW, IR )

      IF ( IONE .NE. 3REQU  ) GO TO 1120
      IF ( ITWO . EQ. 3REND )   GO TO 2000
      JK = NFIND ( KNOD )
      DO 560 K = 1, 4
      KX = LTEMP (K)
      IF ( KX . EQ. 0 )  GO TO 560
      IF ( ITWO . NE . 3RRES ) GO TO 470
C**** STORE RESERVOIR EQUATIONS FOR CAPACITY AND AREA AS FUNCTIONS OF
C**** WATER SURFACE ELEVATION
      RDATA ( JK, KX) = CTEMP (K)
      GO TO 560
  470 IF ( ITWO . NE. 3RSED ) GO TO 480
C**** STORE EQUATIONS FOR SEDIMENT INFLOW COMPUTATIONS
      RDATA ( JK, KX) = CTEMP (K)
      GO TO 560
  480 IF ( ITWO . NE. 3RTWR )  GO TO 490
C**** STORE EQUATIONS WHERE TAILWATER ELEVATION IS FUNCTION OF DISCHARGE
      TDATA ( JK, KX) = CTEMP (K)
      GO TO 560
  490 IF ( ITWO . NE. 3REFF ) GO TO 500
C**** STORE EQUATIONS OF HORSEPOWER AND DISCHARGE ( AT FULL GATE)
C**** AS FUNCTIONS OF NET HEAD
      ENERGY ( JK, KX) = CTEMP (K)
      GO TO 560
  500 IF ( ITWO . NE. 3RCAP ) GO TO 510
C**** STORE CONSTRAINTS CONCERNING TURBINE CAPABILITIES
      CAPBAB (JK, KX) = CTEMP (K)
      GO TO 560
  510 IF ( ITWO . NE. 3RPOW ) GO TO 520
C**** STORE FIRM POWER REQUIREMENTS IN TERMS OF KILOWATT-HOURS PER TIME
C**** FRAME
      PDATA ( JK, KX) = CTEMP (K)
      GO TO 560
  520 IF ( ITWO .NE. 3RRUL ) GO TO 530
C**** STORE TARGET LEVELS FOR RESERVOIR IN TERMS OF CAPACITIES OR
C**** WATER SURFACE ELEVATIONS
      RULE ( JK, KX) = CTEMP (K)
      IF ( KX. EQ. 12 ) RULE ( JK, 13 ) = CTEMP (5)
      GO TO 560
  530 IF ( ITWO . NE . 3REVP )  GO TO 540
C**** STORE RESERVOIR EVAPORATION COEFFICIENTS IN UNITS OF FEET PER
C**** ACRE OF RESERVOIR AREA
      CONEVP ( JK, KX) = CTEMP (K)
      GO TO 560
  540 IF ( ITWO . NE. 3RBNK ) GO TO 1140
C**** STORE COEFFICIENTS FOR BANK STORAGE IN TERMS OF CHANGE IN STORAGE
C**** PER TIME FRAME
      BANKCO ( JK) = CTEMP (K)
  560 CONTINUE
```

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      SUBROUTINE PERUSE (JREAD , IW, IR )

      GO TO 450
C**** READ AND STORE INFLOW, DEMAND, AND CONSUMPTIVE USE CARDS FOR FIRST
C**** TIME FRAME ONLY WHERE TITLE CARDS MUST PRECEDE DATA CARDS
  600 IF ( JREAD . GT. 4 )  GO TO 650
      READ ( IR , 230 ) IONE , ITWO , ( LTEMP (K) , K = 1, 11  )
      WRITE ( IW, 240 ) IONE , ITWO, ( LTEMP (K) , K= 1, 11 )
      IF ( IONE . EQ. 3REND )  GO TO 2000
      IF ( IONE . NE. 3RSUR )  GO TO 1180
      JK = NFIND ( LTEMP (2) )
      IS = LTEMP (1)
      IF ( ITWO . NE. 3RDEM ) GO TO 620
C**** STORE TITLE OF DEMAND OR DIVERSION REQUIREMENT
      DO 610 K = 1, 8
      KX = K + 3
      KDEMNM ( JK, IS, K) = LTEMP (KX)
  610 CONTINUE
      GO TO 650
C**** STORE TITLE OF INFLOW SOURCE
  620 DO 630 K= 1, 8
      KX = K + 3
      KQINNM ( JK, IS, K ) = LTEMP (KX)
  630 CONTINUE
C**** READ AND STORE INFLOW . DEMAND AND CONSUMPTIVE USE DATA AS WELL AS
C**** TRANSACTION CARDS ( USED FOR BOTH JREAD = 4 AND 5 )
  650 READ  (IR, 290) IONE, ITWO, (LTEMP(I), I = 1, 4), (CTEMP(J), J = 1
     A, 10), (LTEMP(K), K = 5, 7)
      WRITE  (IW, 300) IONE, ITWO, (LTEMP(I), I = 1, 4), (CTEMP(J), J =
     A1, 10), (LTEMP(K), K = 5, 7)
      IF ( IONE . EQ. 3REND ) GO TO 2000
      JK = NFIND ( LTEMP (3) )
      IS = LTEMP (1)
      MO = LTEMP (5)
C**** RAISE MAGNITUDE OF DEMAND BY POWER OF 10 ( LTEMP (6) )
      NEXP = LTEMP (6)
      FAC = 10.0 ** NEXP
      CTEMP (1) = CTEMP (1) * FAC
      IF ( IONE . NE. 3RDEM )  GO TO 700
C**** STORE DEMAND DATA WITH OR WITHOUT REQUIRED CONSUMPTIVE USE DATA
      DEMAND ( JK, IS, MO ) = CTEMP (1)
C**** STORE SOURCE INDICATOR IN LOCATION 13 OF DEMAND ARRAY
C**** SYMBOLICALLY THERE ARE ONLY TWO SOURCES SUPPLYING DEMANDS
C**** NAMELY , SURFACE AND SUBSURFACE SOURCES
      IF ( ITWO . EQ. 3RSUR ) DEMAND ( JK, IS, 13 ) = 1.0
      IF ( ITWO . EQ. 3RGWR ) DEMAND ( JK, IS, 13 ) = 2.0
C**** IN LOCATION 14 OF THE DEMAND ARRAY IS STORED THE USE IE IRRIGATION
C**** OR MUNICIPAL AND INDUSTRIAL OR THE DESTINATION IN A TRANSFER OF
C**** FLOWS FROM FACILITY TO FACILITY
      IF ( LTEMP (4) . EQ. 3RIRR ) DEMAND ( JK, IS, 14 ) = 1.0
      IF ( LTEMP (4) . EQ. 3RMAI ) DEMAND ( JK, IS, 14 ) = 2.0
      SUBROUTINE PERUSE (JREAD , IW, IR )

      IF ( LTEMP (4) . EQ. 3RGWV ) DEMAND ( JK, IS, 14 ) = 4.0
      IF ( LTEMP (4) . EQ. 3RSUR ) DEMAND ( JK, IS, 14 ) = 5.0
      IF ( LTEMP (4) . EQ. 3ROUT ) DEMAND ( JK, IS, 14 ) = 6.0
C**** LTEMP (2) CONTAINS INDICATOR DESIGNATING CONSUMPTIVE USE DATA
C**** OR TRANSFER DATA WILL OR WILL NOT FOLLOW DEMAND CARD
      IF ( LTEMP (2) .NE. 1 )  GO TO 600
      READ ( IR, 660 ) ICHK,(LTEMP(K),K=1,2),(CTEMP(KA),KA=1,3),
     1            (LTEMP (KB) , KB = 3, 16 )
  660 FORMAT ( R6, I3, I2, F9.0, 2F3.0, 3 ( R3, I3, I2, I3) , 16X, I2 ,
     1          1X, I2 )
      WRITE ( IW, 670) ICHK,(LTEMP(K),K=1,2),(CTEMP(KA),KA=1,3),
     1            (LTEMP (KB) , KB = 3, 16 )
  670 FORMAT(1H ,R6,I3,I2, F9.0, 2F3.0, 3 ( R3, I3, I2, I3) , 16X, I2 ,
     1          1X, I2 )
C**** CONSUMPTIVE USE OR TRANSFER DATA WILL BE READ AND STORED
      IF ( ICHK . NE. 6RCONUSE )  GO TO 1160
      JK = NFIND ( LTEMP (1) )
      IS = LTEMP (2)
      MO = LTEMP ( 15)
      CONUSE ( JK, IS, MO ) = CTEMP (1)
      CONUSE ( JK, IS, 13 ) = CTEMP (2)
      CONUSE ( JK, IS, 14 ) = CTEMP (3)
      DO 680 K = 3, 14
      KA = K + 16
      KUSE ( JK, IS, KA ) = LTEMP (K)
  680 CONTINUE
      GO TO 600
  700 IF ( IONE . NE. 3RQIN )  GO TO 740
C**** STORE INFLOW DATA WITH OR WITHOUT BREAKDOWN OF CHEMICAL
C**** CONSTITUENTS - LTEMP (2) DESIGNATES UNITS OF INPUT I.E. 1 = MEQ/
C**** LITER AND 2 = PPM
C**** LOCATION 11 IN THE QINFLO ARRAY DESIGNATES THE DESTINATION OF
C**** THE PARTICULAR SOURCE
      IF ( LTEMP (4) .EQ. 3RSUR )  QINFLO (JK, IS, 11 ) = 1.0
      IF ( LTEMP (4) .EQ. 3RGWR )  QINFLO (JK, IS, 11 ) = 2.0
      IF ( LTEMP (4) .EQ. 3RGWV )  QINFLO (JK, IS, 11 ) = 3.0
      IF ( LTEMP (4) .EQ. 3RCHK )  QINFLO (JK, IS, 11 ) = 4.0
      DO 710 K = 1, 10
      QINFLO (JK, IS, K ) = 0.0
  710 CONTINUE
      IF ( CTEMP (1) . LE. 0.0 )  GO TO 600
      QINFLO (JK, IS, 1 ) = CTEMP (1)
C**** CHECK TO DETERMINE IF DATA CONCERNING CHEMICAL CONSTITUENTS
C**** ARE PART OF THIS DATA
      IF ( CTEMP (2) . GT. 0.0 ) GO TO 720
C**** CARD DOES NOT CONTAIN DATA FOR CHEMICAL CONSTITUENTS
      QINFLO ( JK, IS, 10) = CTEMP (10)
      GO TO 600
C**** CARD CONTAINS DATA FOR CHEMICAL CONSTITUENTS
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      SUBROUTINE PERUSE (JREAD , IW, IR )

      DO 730 K = 2, 10
      QINFLO (JK, IS, K ) = CTEMP (K)
  730 CONTINUE
      QINFLO ( JK, IS, 12 ) = LTEMP (2)
      GO TO 600
  740 IF ( IONE . NE. 3RTRN )  GO TO 1200
C**** STORE DATA IN TRANSACTION CARDS *** ONLY ONE VARIABLE OR PARAMETER
C**** CHANGE CAN BE ACCOMMODATED PER CARD
      KA = CTEMP (1)
      IF ( ITWO . NE. 3RRES )  GO TO 750
      RDATA ( JK, KA ) = CTEMP (2)
      GO TO 600
  750 IF ( ITWO . NE. 3RTDA )  GO TO 760
      TDATA ( JK, KA) = CTEMP (2)
      GO TO 600
  760 IF ( ITWO . NE. 3RPDA )  GO TO 770
      PDATA ( JK, KA) = CTEMP (2)
      GO TO 600
  770 IF ( ITWO . NE. 3RENE )  GO TO 780
      ENERGY ( JK, KA ) = CTEMP (2)
      GO TO 600
  780 IF ( ITWO . NE. 3RCAP )  GO TO 790
      CAPRAB ( JK, KA) = CTEMP (2)
      GO TO 600
  790 IF ( ITWO . NE. 3RBNK )  GO TO 800
      BANKCO (JK) = CTEMP (2)
      GO TO 600
  800 IF ( ITWO . NE. 3REVP )  GO TO 810
      CONEVP ( JK, KA) = CTEMP (2)
      GO TO 600
  810 IF ( ITWO . NE. 3RRUL )  GO TO 1200
      RULE ( JK, KA) = CTEMP (2)
      GO TO 600
C**** ALL PROGRAM CONTROLLED ERROR MESSAGES ARE GENERATED HERE
 1000 WRITE ( IW, 1010 )
 1010 FORMAT ( 1H1, 7X, 26HTHIS IS NOT A CONTROL CARD  )
      CALL EXIT
 1020 WRITE ( IW , 1030 )
 1030 FORMAT ( 1H1, 7X, 36HNUMBER OF SEQUENCE POINTS EXCEEDS 20 )
      CALL EXIT
 1040 WRITE ( IW , 1050 )
 1050 FORMAT ( 1H1, 7X, 36HNO END SIGNAL FOUND FOR CONTROL DATA  )
      CALL EXIT
 1060 WRITE ( IW , 1070 )
 1070 FORMAT ( 1H1, 8X, 33HRESERVOIR CHEMISTRY CARD MISSING   )
      CALL EXIT
 1080 WRITE ( IW , 1090 )
 1090 FORMAT ( 1H1, 7X, 34HDATA FOR JREAD = 3 IS OUT OF ORDER )
      CALL EXIT
      SUBROUTINE PERUSE (JREAD , IW, IR )

 1110 FORMAT ( 1H1, 7X, 29HSOIL COLUMN DATA OUT OF ORDER  )
      CALL EXIT
 1120 WRITE ( IW, 1130 )
 1130 FORMAT ( 1H1, 7X, 28HEQUATION CARDS OUT OF ORDER   )
      CALL EXIT
 1140 WRITE ( IW, 1150 )
 1150 FORMAT ( 1H1, 7X, 34HITWO INDEX NOT FOUND IN VALID LIST )
      CALL EXIT
 1160 WRITE ( IW , 1170)
 1170 FORMAT ( 1H1, 8X, 30HNO CONSUMPTIVE USE CARD FOUND  )
      CALL EXIT
 1180 WRITE ( IW , 1190 )
 1190 FORMAT ( 1H1, 7X, 3[illegible]INFLOW OR DEMAND CARDS ARE OUT OF ORDER  )
      CALL EXIT
 1200 WRITE ( IW, 1210 )
 1210 FORMAT ( 1H1, 7X, 34HTRANSACTION CARDS ARE OUT OF ORDER  )
      CALL EXIT
 1220 WRITE (IW , 1230 )
 1230 FORMAT ( 1H1, 7X, 34HDATA FOR JREAD = 2 IS OUT OF ORDER )
      CALL EXIT
 2000 RETURN
      END
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   SUBROUTINE WRIT ( MO, IYR , IW )
C
    COMMON / GENRL / LTITLE(8), NCTPL(20, 3), MOBEG, IYRBEG, MOEND, I
   AYREND, NUMNOD, ISEQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
    COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
   ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
   RDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,8)
    COMMON / POWER / CAPBAB(20, 20), TDATA(20, 4), ENERGY(20, 8), PDA
   ATA(20, 12)
    COMMON / PROPER / SOIL(20, 10, 21), BTANK(20, 10), TTANK(20, 10),
   1 GRTANK(20, 10)   , NSEG (20) , CONUSE (20, 10, 30)
   2             , KUSE (20, 10, 30)
    COMMON / PARAM / BEGRES ( 20, 11 ) , BEGWR ( 20, 10 ) ,
   1          PREDIC ( 20, 10 ) , OBSVAL (20.10), CHEMDM ( 20, 10, 10)
    DIMENSION MON (12) , LTEMP (20 ) , TEMP (10)
    EQUIVALENCE ( CONUSE, KUSE )
    DATA (( MON (K) , K = 1, 12) = 3RJAN, 3RFEB, 3RMAR, 3RAPR, 3RMAY.
   1        3RJUN, 3RJUL, 3RAUG, 3RSEP, 3ROCT, 3RNOV, 3RDEC )
    DATA ( IPAGE = 0 )
    MONTH = MON (MO )
    KYR = IYR + 1900
    DO 700 KN = 1, NUMNOD
    IPAGE = IPAGE + 1
    WRITE ( IW, 50)  (LTITLE (K) , K = 1, 8 ) , IPAGE
 50 FORMAT( 1H1, 7X, 8A8, 3X, 19HNUMBER OF NODES = 3  , 6X,
   1        8HPAGE NO.  , I3 / )
    KNODE = NCTPL (KN,1)
    WRITE ( IW, 60 ) KNODE, MONTH, KYR
 60 FORMAT ( 8X, 14HNODE NUMBER = , I3, 5X, 9HMONTH OF  , R3, 10X,
   1       5HYEAR   , I4 // 58X, 6HVOLUME, 4X, 2HCA , 4X, 2HMG, 4X,
   2       2HNA, 4X, 2HCL, 4X, 3HSO4 , 2X, 4HHCO3 , 3X, 3HCO3 , 3X,
   3       3HNO3 , 3X, 11HTOTAL SALTS / 56X, 9HACRE FEET,
   4       9 (3X, 3HPPM ) , 3X, 7HTONS/AF / )
    WRITE ( IW, 70)
 70 FORMAT ( 8X, 42HOPERATIONAL SEQUENCE OF SURFACE FACILITIES   / )
 95 GO TO ( 100, 110, 130 ) , KN
100 MA = 4
    MB = 5
    MC = 9
    MD = 10
    GO TO 150
110 MA = 2
    MB = 3
    MC = 7
    MD = 8
    GO TO 150
130 MA= 2
    MB = 3
    MC = 5
    MD = 6
150 NS = NUMSEQ ( KN )
```

```
      SUBROUTINE WRIT ( MO, IYR , IW )

      DO 490 KS = 1, NS
      IS = IABS ( ISEQ ( KN, KS ) )
C**** WRITE OUTPUT OF LINES CONTROLLED BY INDEX(MA) (INFLOWS- DEMANDS)
      IF ( KS. GT. MA )  GO TO 190
  160 IF ( ISEQ ( KN, KS ).GT. 0 ) GO TO 450
      IF ( ISEQ ( KN, KS ).LT. 0 )  GO TO 300
      GO TO 490
  190 IF ( KS . NE. MB )  GO TO 220
      WRITE ( IW , 210 )
  210 FORMAT (/8X, 28HOBSERVED OUTFLOWS FROM NODE  / )
  220 IF ( KS. LE. MC )  GO TO 450
      IF ( KS . NE. MD )   GO TO 250
      WRITE ( IW , 230 )
  230 FORMAT (/8X, 40HSUBSURFACE OPERATIONS AND FLOW TRANSFERS  / )
      LTEMP ( 1 ) = 8HAQUIFER
      LTEMP ( 2 ) = 8H CONDITI
      LTEMP ( 3 ) = 8HONS OF L
      LTEMP ( 4 ) = 8HAST TIME
      LTEMP ( 5 ) = 8H FRAME
      DO 240 K = 1, 10
      KA = K + 5
      LTEMP (KA) = BEGWR ( KN, K )
  240 CONTINUE
      TONS = BEGWR ( KN, 10 ) * 1.36E-3
      WRITE( IW, 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
  250 IF ( KS . LE. NS )  GO TO 160
C***** THIS PORTION OF THE SUBROUTINE SETS UP ALL DEMANDS FROM SYSTEM
C*****IN CORRECT OUTPUT MODE
  300 DO 320 K = 1, 5
      LTEMP (K) = KDEMNM ( KN, IS, K )
  320 CONTINUE
      LTEMP (6) = DEMAND ( KN , IS, 16 )
  330 DO 340 K = 2, 10
      KA = K + 5
      LTEMP (KA) = CHEMDM ( KN, IS, K )
  340 CONTINUE
      TONS = CHEMDM (KN, IS, 10 ) * 1.36 E-3
C**** THIS IS THE GENERAL OUTPUT STATEMENT FOR MOST OF THE OUTPUT
  400 IF ( MARK .GT. 0 )  GO TO 408
      IF ( LTEMP (6) .GT. 0 )  GO TO 408
      TONS= 0.0
      DO 405 K = 6, 15
      LTEMP (K) = 0
  405 CONTINUE
  408 WRITE ( IW, 410 ) ( LTEMP (K) , K = 1, 15 ) , TONS
  410 FORMAT ( 11X, 5A8 , 5X, I9, 8 (2X, I4) , 2X, I5, 3X, F6.3 )
      IF ( ISEQ ( KN, KS ) . GT. 0 ) GO TO 490
      IF ( DEMAND ( KN, IS, 14 ) . GT. 2.0 ) GO TO 490
C**** THIS PORTION OF THE SUBROUTINE COMPUTES AND OUTPUTS THE SHORTAGES
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      SUBROUTINE WRIT ( MO, IYR , IW )

      KTEM = DEMAND ( KN , IS, MO )
      LTEMP (17) = KTEM - LTEMP (6)
      WRITE ( IW, 420 ) LTEMP (17 )
  420 FORMAT ( 11X, 31HSHORTAGE FROM THE IDEAL DEMAND   , 14X, I9  )
      GO TO 490
C**** THIS PORTION OF THE ROUTINE SETS UP ALL INFLOWS TO THE
C**** SYSTEM IN THE CORRECT OUTPUT MODE
  450 DO 460 K = 1, 5
      LTEMP (K) = KOINNM ( KN, IS , K )
  460 CONTINUE
      LTEMP (6) = QINFLO ( KN, IS , 1 )
      DO 470 K = 2, 10
      KA = K + 5
      LTEMP (KA) = QINFLO ( KN, IS, K )
  470 CONTINUE
      TONS = QINFLO ( KN, IS, 10) * 1.36E-3
      GO TO 400
  490 CONTINUE
C**** BEGIN THE COMPARISON OF OBSERVED AND PREDICTED END OF NODE
C**** FLOWS AND CHEMISTRY
  500 WRITE ( IW , 520 )
  520 FORMAT ( // 8X, 16HCOMPARISON INDEX    / )
      LTEMP ( 1) = 8HTOTAL OB
      LTEMP ( 2) = 8HSERVED O
      LTEMP ( 3) = 8HUTFLOWS
      LTEMP ( 4) = 8HFROM NOD
      LTEMP ( 5) = 8HE
      DO 530 K = 1, 10
      KA = K + 5
      LTEMP (KA ) = OBSVAL ( KN , K )
  530 CONTINUE
      TONS = OBSVAL ( KN, 10 ) * 1.36E-3
      WRITE ( IW , 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
      LTEMP (1) = 8HPREDICTE
      LTEMP ( 2) = 8HD OUTFLO
      LTEMP ( 3) = 8HW FROM T
      LTEMP ( 4) = 8HHIS NODE
      LTEMP ( 5) = 8H
      DO 540 K = 1, 10
      KA = K + 5
      LTEMP (KA ) = PREDIC ( KN, K )
  540 CONTINUE
      TONS = PREDIC ( KN , 10 ) * 1.36E-3
      WRITE ( IW , 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
      LTEMP ( 1) = 8HSIMPLE D
      LTEMP ( 2) = 8HIFFERENC
      LTEMP ( 3) = 8HF (OBSER
      LTEMP ( 4) = 8HVED - PR
      LTEMP ( 5) = 8HEDICTED)
      SUBROUTINE WRIT ( MO, IYR , IW )

      TEMP (K) = OBSVAL (KN, K ) - PREDIC ( KN, K )
      KA = K+ 5
      LTEMP (KA ) = TEMP (K)
  550 CONTINUE
      TONS = TEMP (10) * 1.36E-3
      WRITE ( IW , 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
      WRITE ( IW, 560)
  560 FORMAT ( / 8X, 25HCHEMICAL CHANGES IN NODE  / )
      LTEMP (1) = 8HOBSERVED
      LTEMP (2) = 8H CHANGE
      DO 570 K = 3, 5
      LTEMP (K) = 8H
  570 CONTINUE
      DO 580 K = 1, 10
      TEMP (K) = OBSVAL ( KN, K ) - QINFLO (KN, 1, K )
      KA = K + 5
      LTEMP (KA) = TEMP (K)
  580 CONTINUE
      TONS = TEMP (10) * 1.36E-3
      LTEMP (6) = 0
      WRITE ( IW , 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
      LTEMP (1) = 8HPREDICTE
      LTEMP (2) = 8HD CHANGE
      DO 590 K = 1, 10
      TEMP (K) = PREDIC (KN, K ) - QINFLO (KN, 1, K )
      KA = K + 5
      LTEMP (KA) = TEMP (K)
  590 CONTINUE
      LTEMP (6) = 0
      TONS = TEMP (10) * 1.36E-3
      WRITE ( IW , 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
      IF ( KN . NE. NUMNOD )   GO TO 700
      WRITE ( IW, 600 )
  600 FORMAT ( / 8X, 26HCHEMICAL CHANGES IN SYSTEM  / )
      LTEMP (1) = 8HOBSERVED
      LTEMP (2) = 8H CHANGE
      DO 610 K = 1, 10
      TEMP (K) = OBSVAL ( KN, K ) - QINFLO (1, 1, K)
      KA = K + 5
      LTEMP (KA ) = TEMP (K)
  610 CONTINUE
      LTEMP (6) = 0
      TONS = TEMP (10 ) * 1.36E-3
      WRITE ( IW , 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
      LTEMP (1) = 8HPREDICTE
      LTEMP (2) = 8HD CHANGE
      DO 620 K = 1, 10
      TEMP (K) = PREDIC (KN, K ) - QINFLO (1, 1, K )
      KA = K + 5
      SUBROUTINE WRIT ( MO, IYR , IW )

  620 CONTINUE
      LTEMP (6) = 0
      TONS = TEMP (10 ) * 1.36E-3
      WRITE ( IW , 410 )  (LTEMP (K) , K = 1, 15 ) , TONS
  700 CONTINUE
 2000 RETURN
      END
      SUBROUTINE RESOPR ( QFLOW , KN, MO, IW )

        COMMON / GENRL / LTITLE(8), NCTPL(20, 5), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMNOD, ISEQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
        COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     BDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,8)
        COMMON / POWER / CAPBAB(20, 20), TDATA(20, 4), ENERGY(20, 8), PDA
     ATA(20, 12)
       COMMON / PARAM / BEGRES ( 20, 11 ) , REGWR ( 20, 10 ) ,
     1         PREDIC ( 20, 10 ) , OBSVAL (20,10), CHEMDW ( 20, 10, 10)
       DIMENSION IDAYS ( 12) , MODE (20), PREL (20 ), PRFCAP ( 20) ,
     1         PARFA ( 20 ) , QFLOW (10) , CF (10 )
       DATA ((IDAYS(K),K=1,12) = 31,28,31,30,31,30,31,31,30,31,30,31)
       DATA ( IMON = 0) , ( CONST = 1.983471) , ( IFIR = 0 )  ,
     1        ( EPSLON = 1.0E1 )
C**** THIS SUBROUTINE SIMULATES THE OPERATION OF A RESERVOIR WITH OR
C**** WITHOUT A POWER PLANT - ASSUMES CHEMISTRY MIX ( LINEAR) FOR EVERY
C**** INFLOW IE WHEN QFLOW (1) IS GREATER THAN ZERO . HOWEVER, THE
C**** UPDATE IS SIMULATED ONCF PER MONTHLY TIME FRAME.  THE SEDIMENT
C**** INFLOW AND INCREMENTAL DEPOSIT IS COMPUTED DURING THE INITIAL
C**** ITERATION ONLY. THIS ASSUMES THAT SUBSEQUENT INFLOWS ARE FROM
C**** UPSTREAM RESERVOIR RELEASES AND CONSIDERED SEDIMENT FREE . THE
C**** MINIMUM RESERVOIR CAPACITY IS INCREASED AT THE BEGINNING OF FACH
C**** TIME FRAME ON THE BASIS OF THE SEDIMENT DEPOSITED IN THE PREVIOUS
C**** TIME FRAME. IN THE ARGUMENT LIST - QFLOW IS AN ARRAY CONTAINING
C**** VOLUMF AND CHEMISTRY OF RESERVOIF INFLOW OR OUTFLOW, KN = NODE
C**** INDEX, MO = MONTH , IW = LOGICAL WRITE UNIT
      KNODE = NCTPL ( KN, 1)
      IF ( IFIR . NF. 0 )  GO TO 20
      DO 10 J = 1, 20
      DO 10 K = 1, 11
      BEGRES ( J, K) = 0.0
   10 CONTINUE
      IFIR = 1
C**** CHECK TO DETEPMINE IF THIS IS THE FIRST CALL FOR ANY RESERVOIR
C**** IN THIS TIMF FRAMF
   20 IF ( IMON . EQ. MO )  GO TO 35
C**** INITIALIZE CALL COUNTERS FOR ALL RESERVOIRS
      DO 30 K = 1, 20
      MODE (K) = 0
   30 CONTINUE
      DAYS = IDAYS (MO)
      IMON = MO
C**** CHECK TO DETERMINE IF THIS IS THE INTITIAL CALL FOR THIS
C**** RESERVOIR IF SO UPDATE RESERVOIR CHEMISTRY AND SEDIMFNT
   35 IF ( MODE (KN) . NE. 0 )   GO TO 100
C**** STORE RESERVOIR CHEMISTRY OF PREVIOUS TIME FRAME
      DO 40 K = 2, 10
      KA = K + 99
      BEGRES (KN, K) = RDATA ( KN , KA )
      SUBROUTINE RESOPR ( QFLOW , KN, MO, IW )

      BEGRES ( KN, 1 ) = RDATA (KN, 3 )
C**** UPDATE MINIMUM RESERVOIR CAPACITY ON BASIS OF SEDIMENT DEPOSITED
C**** DURING PREVIOUS TIME FRAME
      RDATA ( KN, 12) = RDATA ( KN, 12 ) + BEGRES ( KN, 11 )
C**** UPDATE TOTAL SEDIMENT DEPOSITED
      RDATA ( KN, 20) = RDATA ( KN, 20 ) + BEGRES ( KN, 11 )
C**** DURING INITIAL ITERATION QFLOW (1) MUST EQUAL TO OR GREATER THAN
C**** ZERO ( MUST NOT REPRESENT A RELEASE )
      IF ( QFLOW (1) . LT. 0.0 ) GO TO 1000
C**** COMPUTE SEDIMENT INFLOW AS A FUNCTION OF WATER INFLOW WHERE
C**** QSED (TONS/DAY) = A * QCFS ** B
      QSED = 0.0
      A = RDATA (KN, 15)
C**** CHECK TO DETERMINE IF SEDIMENT IS TO BE CONSIDERED FOR THIS
C**** RESERVOIR
      IF ( A . EQ. 0.0 )    GO TO 60
      IF ( QFLOW (1) . EQ. 0.0 )  GO TO 60
      B = RDATA ( KN, 16)
      QCFS = QFLOW (1) / CONST/ DAYS
C**** TEST TO DETERMINE IF THERE ARE TWO FUNCTIONS FOR SEDIMENT AND
C**** WHICH OF THE TWO IS REQUIRED FOR THE SEDIMENT COMPUTATION
      IF ( QCFS . LT. RDATA (KN, 19 ) ) GO TO 50
      A = RDATA (KN, 17)
      B = RDATA (KN, 18 )
   50 QSED = A * QCFS ** B
C**** CONVERT FROM TONS PER DAY TO ACRE FEET PER MONTH
      QSED = QSED * DAYS * 6.1218E-4
   60 BEGRES ( KN, 11 ) = QSED
C**** CHECK TO DETERMINE IF RESERVOIR AREA AND WATER SURFACE ELEVATION
C**** ARE INITIALIZED
      IF ( RDATA ( KN, 4 ) . GT. 0.0 )  GO TO 80
      CAP = RDATA (KN, 3 )
      IF ( CAP . LE. 0.0 )  GO TO 1020
      RDATA (KN, 4) = RESEL ( CAP, AREA, KN, IW )
      RDATA (KN, 5) = AREA
C**** INITIALIZE RESERVOIR EVAPORATION, CHANGE IN BANK STORAGE, SPILL,
C**** RELEASE THROUGH OUTLETS AND TURBINES AND TOTAL RELEASE
   80 DO 90 K = 6, 10
      RDATA (KN, K ) = 0.0
   90 CONTINUE
C**** STORE RESERVOIR CAPACITY, WATER SURFACE ELEVATION AND AREA AT
C**** END OF LAST TIME FRAME AS INITIAL VALUES FOR THIS TIME FRAME
      PRECAP (KN) = RDATA (KN, 3)
      PREL (KN) = RDATA (KN, 4)
      PAREA (KN) = RDATA (KN, 5)
C**** SET TARGET CAPACITY FOR THIS RESERVOIR FOR THIS TIME FRAME
C**** THESE TARGET CAPACITIES ARE READ IN AS RULE CURVES.
  100 TARGET = RULE ( KN, MO )
C**** IF TARGET LEVEL IS IN TERMS OF WATER SURFACE ELEVATION FIND
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      SUBROUTINE RESOPR ( QFLOW , KN, MO, IW )

      IF ( RULE (KN, 13) . GT. 0.0 )  TARGET = RESCAP ( TARGET, KN, IW)
C**** THE RESERVOIR OPERATION SUBROUTINE IS DESIGNED ESSENTIALLY
C**** ON THE BASIS OF THREE CONDINTIONS, NAMELY. (1) ON THE FIRST
C**** CALL TO STORE RIVER INFLOW AND TO MAINTAIN THE RESERVOIR
C**** WATER SURFACE LEVEL AT THE TARGET LEVEL, ON SUBSEQUENT CALLS
C**** TO (2) MAKE RELEASES TO SATISFY A DOWNSTREAM REQUIREMENT AND
C**** THEN (3) TO PASS THROUGH A RELEASE FROM AN UPSTREAM RESERVOIR
C**** AS IT MOVES DOWN THROUGH THE SYSTEM TO MEET A DOWNSTREAM DEFICIT
C**** COMPUTATIONS FOR EACH CALL TO THIS SUBROUTINE FOR EACH RESERVOIR
C**** BEGIN HERE. MODE (KN) IS THE COUNTER OF THE NUMBER OF CALLS PER
C**** FRAME FOR EACH RESERVOIR. SET ALL RESERVOIR OPERATION CONSTRAINTS
C**** AT THIS POINT
      TEMCAP = RDATA (KN, 3 )
      EVAP   = RDATA ( KN , 6)
      BSTOR  = RDATA ( KN , 7)
      SPILL  = RDATA ( KN , 8)
      CAPMAX = RDATA ( KN ,11)
      CAPMIN = RDATA ( KN ,12)
      RELMAX = RDATA ( KN ,13)
      RELMIN = RDATA ( KN ,14)
C**** DETERMINE MAGNITUDE OF INFLOW (QFLOW(1)) - IF LESS THAN ZERO
C**** IT REPRESENTS A RELEASE IS TO BE ATTEMPTED FROM THIS RESERVOIR
C**** TO MEET A DOWNSTREAM REQUIREMENT - IF EQUAL OR GREATER THAN
C**** ZERO IT REPRESENTS AN INFLOW TO THIS RESERVOIR - ALL INFLOWS
C**** WILL CHANGE THE CHEMISTRY OF THE RESERVOIR FOR THIS TIME FRAME.
      IF ( QFLOW (1) . EQ. 0.0 )  GO TO 2000
      IF ( QFLOW (1) . LT. 0.0  ) GO TO  700
C**** THIS IS AN INFLOW TO THE RESERVOIR - MIX RESERVOIR CHEMISTRY
C**** WITH RIVER (INFLOW) CHEMISTRY
      CALL CHEMRR ( QFLOW, 0., KN, 1 )
      IF ( MODE (KN) .NE. 0 )  GO TO 600
C**** THIS IS THE FIRST CALL FOR THIS RESERVOIR IN THIS TIME FRAME
C**** AND REPRESENTS CONDITION (1) - SET STORAGE ( STORAF) AND RELEASE
C**** ( REALF ) AS INITIAL VALUES IN ACRE FEET
      STORAF = QFLOW (1)
      RELAF = RELMIN * CONST * DAYS
C**** COMPUTE A SEED FOR RESERVOIR CAPACITY TO START ITERATIVE SCHEME
C**** TO BALANCE RESERVOIR BUDGET - LET NITER = NUMBER OF ITERATIONS
C**** REQUIRED TO OBTAIN BALANCE
      CAPX = TEMCAP + STORAF - RELAF
  200 NITER = 0
  210 NITER = NITER + 1
C**** COMPARE SEED CAPACITY WITH TARGET CAPACITY
      IF ( CAPX . LE. TARGET ) GO TO 220
C**** SEED CAPACITY IS GREATER THAN TARGET CAPACITY - INCREASE RELEASE
      DELTAF = CAPX - TARGET
      RELAF = RELAF + DELTAF
C**** SET CAPACITY EQUAL TO TARGET CAPACITY
      CAPX = TARGET
      SUBROUTINE RESOPR ( QFLOW . KN, MO, IW )

C**** RELEASE
  220 RELCFS = RELAF / CONST / DAYS
      IF ( RELCFS . LE. RELMAX )   GO TO 240
C**** RELEASE IS GREATER THAN MAXIMUM SET RELEASE EQUAL TO MAXIMUM
      RELCFS = RELMAX
      RELAF = RELCFS * CONST * DAYS
      MARK = 1
C**** COMPARE CAPACITY WITH MAXIMUM CAPACITY
  240 IF ( CAPX . LE. CAPMAX ) GO TO 260
C**** CAPACITY IS GREATER THAN MAXIMUM CAPACITY INCREASE RELEASE IF
C**** POSSIBLE AND SET CAPACITY EQUAL TO MAXIMUM CAPACITY
      DELTAF = CAPX - CAPMAX
      CAPX = CAPMAX
      IF ( MARK . EQ. 1 )  GO TO 280
      RELAF = RELAF + DELTAF
      GO TO 220
C**** COMPARE CAPACITY WITH MINIMUM CAPACITY
  260 IF ( CAPX .GE. CAPMIN ) GO TO 300
C**** CAPACITY IS LESS THAN MINIMUM CAPACITY DECREASE RELEASE
      DELTAF = CAPMIN - CAPX
      RELAF = RELAF - DELTAF
      RELCFS = RELAF / CONST / DAYS
C**** SET CAPACITY TO MINIMUM CAPACITY
      CAPX = CAPMIN
C**** COMPARE REDUCED RELEASE WITH MINIMUM RELEASE
      IF ( RELCFS .GE. RELMIN )   GO TO 300
C**** IF MORE THAN TWO ITERATIONS HAVE BEEN MADE AND THE RELEASE IS
C**** LESS THAN MINIMUM RELEASE HALT COMPUTATIONS AS A PROGRAM
C**** CONTROLLED ERROR
      IF ( NITER . LT. 3 ) GO TO 300
      GO TO 1040
C**** CAPACITY AND RELEASE ARE AT MAXIMUM - SET SPILL
  280 SPILL = DELTAF
C**** COMPUTE RESERVOIR EVAPORATION (EVAP) AND CHANGE IN BANK STORAGE
C**** ( BSTOR )  ( IF APPLICABLE )
  300 ELEV = RESEL ( CAPX, AREA . KN, IW )
      EVAP = ( AREA + PAREA (KN) )  * 5.0E-1 * CONEVP (KN)
      BSTOR = 0.0
      IF ( BANKCO (KN) . LE. 0.0 ) GO TO 320
      BSTOR = ( CAPX - PRECAP (KN) ) * BANKCO (KN)
C**** REFINE SEED FOR CAPACITY
  320 CAPY = TEMCAP + STORAF - RELAF - EVAP - BSTOR
C**** CHECK FOR CONVERGENCE LIMIT OR BALANCED RESERVOIR BUDGET
      DIFF = ABS ( CAPX - CAPY )
      IF ( DIFF .LE. EPSLON ) GO TO 350
C**** RESERVOIR NOT IN BALANCE RESET SEED START NEW ITERATION--
C**** CHECK NUMBER OF ITERATIONS AGAINST LIMIT
      IF ( NITER . GT. 10 ) GO TO 1060
      CAPX = CAPY
      SUBROUTINE RESOPR ( QFLOW , KN, MO, IW )

C**** RESERVOIR BUDGET IS BALANCED RESET RDATA ARRAY
  350 RDATA (KN , 3 ) = CAPX
      RDATA (KN , 4 ) = ELEV
      RDATA (KN , 5 ) = AREA
      RDATA (KN , 6 ) = EVAP
      RDATA (KN , 7 ) = BSTOR
      RDATA (KN , 8 ) = SPILL
      RDATA (KN , 9 ) = RELAF
      RDATA (KN ,10 ) = RELAF + SPILL
C**** SET VOLUME AND CHEMISTRY OF FLOW IN RIVER (QFLOW) BELOW
C**** RESERVOIR
  400 IF ( RDATA (KN, 10) .LE. 0.0 ) GO TO 440
      DO 420 K = 2, 10
      QFLOW (K) = BEGRES (K)
  420 CONTINUE
      QFLOW (1) = RDATA ( KN, 10 )
      GO TO 480
C**** RESERVOIR RELEASE EQUALS ZERO - SET QFLOW ARRAY EQUAL TO ZERO
  440 DO 460 K = 1, 10
      QFLOW (K) = 0.0
  460 CONTINUE
C**** CHECK TO DETERMINE IF POWER FACILITIES ARE PART OF RESERVOIR
C**** COMPLEX
  480 IF ( CAPBAB (KN, 1) . LT. 1.0 )  GO TO 2000
C**** POWER FACILITITES ARE WITHIN THE COMPLEX- COMPUTE AVERAGE
C**** WATER SURFACE ELEVATION IN THE RESERVOIR FOR THIS TIME FRAME
      ELEV = ( RDATA ( KN, 4) + PREL (KN) ) * 5.0E-1
      CALL PWROPR ( RELCFS, KN, MO, DAYS, ELEV, SPILL, IW )
      GO TO 2000
C**** THIS INFLOW IS TO PASS THROUGH THIS RESERVOIR AS A RELEASE
C**** FROM AN UPSTREAM RESERVOIR TO MEET A DOWNSTREAM DEFICIT
C**** (CONDITION (3) .
C**** CHECK TO DETERMINE IF THIS RESERVOIR IS SPILLING
  600 IF ( SPILL . LE. 0.0 )  GO TO 640
C**** RESERVOIR IS SPILLING ADD INFLOW TO SPILL
      SPILL = SPILL + QFLOW (1)
      RDATA (KN, 8) = SPILL
C**** UPDATE TOTAL RELEASE
      RDATA (KN, 10) = RDATA (KN, 10) + QFLOW (1)
  620 RELCFS = RDATA (KN, 9) / CONST / DAYS
      GO TO 400
C**** RESERVOIR IS NOT SPILLING INCREASE RELEASE THROUGH OUTLET WORKS
C**** AND TURBINES BY ADDING INFLOW
  640 RELAF = RDATA (KN, 9 ) + QFLOW (1)
      RELCFS = RELAF / CONST / DAYS
C**** COMPARE THIS RELEASE WITH MAXIMUM RELEASE
      IF ( RELCFS . GT. RELMAX )  GO TO 660
C**** RELEASE DOES EXCEED MAXIMUM RELEASE
      RDATA (KN, 9 ) = RELAF
      SUBROUTINE RESOPR ( QFLOW , KN, MO, IW )

      RDATA (KN, 10) = RDATA (KN, 9 ) + RDATA (KN, 8 )
      GO TO 400
C**** RELEASE EXCEEDS MAXIMUM RELEASE SET RELEASE EQUAL TO MAXIMUM
C**** RELEASE AND ENTER ITERATIVE SCHEME
  660 RELAF = RELMAX * CONST * DAYS
      STORAF = QFLOW (1) - RELAF
C**** SET SEED CAPACITY FOR ITERATIVE SCHEME
  680 CAPX = TEMCAP + EVAP + SPILL + BSTOR
      GO TO 200
C**** THIS IS A RELEASE REQUIRED FROM THIS RESERVOIR TO MEET A
C**** DOWNSTREAM REQUIREMENT . CONDITION (2)
  700 RELAF = ABS ( QFLOW (1) )
C**** CHECK CONSTRAINTS TO DETERMINE IF THIS RELEASE IS POSSIBLE
      IF ( SPILL . GT. 0.0 ) GO TO 2000
      IF ( TEMCAP . LE. CAPMIN )  GO TO 2000
C**** RELEASE IS POSSIBLE SET STORAGE AND RELEASE IN ACRE FEET
C**** AND ENTER ITERATIVE SCHEME
      STORAF = 0.0
      GO TO 680
C**** PROGRAM CONTROLLED ERROR MESSAGES ARE GENERATED HERE
 1000 WRITE ( IW , 1010 ) QFLOW (1)
 1010 FORMAT ( 1H1, 7X, 17HINITIAL INFLOW =  , F10.0 , 3X,
     1         21HNEGATIVE INFLOW ERROR     )
      GO TO 1500
 1020 WRITE ( IW, 1030 ) CAP
 1030 FORMAT ( 1H1 , 7X, 11HCAPACITY =  , F10.0 , 3X,
     1           23HNEGATIVE CAPACITY ERROR    )
      GO TO 1500
 1040 WRITE ( IW , 1050) RELCFS
 1050 FORMAT ( 1H1, 7X,10HRELEASE = , F12.1 , 3X, 17HAND IS LESS THAN  ,
     1          15HMINIMUM RELEASE    )
      GO TO 1500
 1060 WRITE ( IW, 1070 ) NITER
 1070 FORMAT ( 1H1, 7X, 44HNUMBER OF ITERATIONS EXCEED LIMIT AND ARE = ,
     1          I3 )
      GO TO 1500
 1500 WRITE ( IW, 1510 ) KNODE , MO, MODE (KN)
 1510 FORMAT ( 8X, 12HIN NODE NO.    , I3, 8HMONTH =  , I3, 5X,
     1           12HCALL NO.  =  , I3, 3X, 18HCOMPUTATION HALTED  )
      CALL EXIT
 2000 RETURN
      END
      FUNCTION RESCAP ( ELEV, KN, IW )
C
C**** THIS FUNCTION IS USED TO COMPUTE RESERVOIR CAPACITIES AS A SECOND
C**** DEGREE POLYNOMIAL WHERE CAPACITY IS A FUNCTION OF ELEVATION
      COMMON / GENRL / LTITLE(8), NCTRL(20, 3), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMNOD, ISEQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
      COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), RA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     BDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,8)
      DIMENSION CA (10)
      DO 10 K = 1, 5
      CA (K) = 0.0
   10 CONTINUE
      DO 30 K = 25, 97, 4
      KX = K
      TEST = RDATA ( KN, K )
      IF ( TEST .EQ. 0.0 )  GO TO 60
      IF ( ELEV . LT. TEST )  GO TO 60
   30 CONTINUE
      NODE = NCTRL (KN, 1 )
      WRITE ( IW, 50 ) NODE , ELEV
   50 FORMAT ( 1H1, 7X, 41HTHE EQUATION ARRAY FOR RESERVOIR IN NODE
     1        I3, 30H WAS EXCEEDED FOR ELEVATION =  ,F10.2 )
      CALL EXIT
   60 KW = KX - 4
      DO 80 K = 1, 3
      KY = KW + K
      CA (K) = RDATA ( KN, KY)
   80 CONTINUE
      X = ELEV
      X = ELEV - RDATA ( KN, KW )
      RESCAP = FOFX ( CA , X, 1 )
      RETURN
      END
      FUNCTION RESEL ( CAP , AREA , KN, IW )

C**** THIS FUNCTION IS USED TO COMPUTE ELEVATION AND AREA FOR
C**** A RESERVOIR ON THE BASIS OF A SECOND DEGREE POLYNOMIAL WHERE
C**** CAPACITY IS A FUNCTION OF ELEVATION AND AREA IS THE FIRST
C**** DERIVATIVE OF THE FUNCTION
        COMMON / GENRL / LTITLE(8), NCTRL(20, 3), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMNOD, ISEQ(20, 20), KPRI, NUMSEC(20), NDWTR(20, 20)
        COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     BDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAGUNM (20,8)
      DIMENSION CF (10)
      DO 50 K = 26, 98, 4
      KX = K
      TEST = RDATA ( KN , K )
      IF ( CAP . LT. TEST )  GO TO 70
      IF ( TEST . EQ. 0.0 )   GO TO 70
   50 CONTINUE
      NODE = NCTRL ( KN, 1 )
      WRITE ( IW, 60 ) NODE , CAP
   60 FORMAT ( 1H1, 7X, 41HTHE EQUATION ARRAY FOR RESERVOIR IN NODE
     1          I3, 30H WAS EXCEEDED FOR CAPACITY OF    , F10.0 )
      CALL EXIT
   70 KW = KX - 1
      DO 90 K = 1, 3
      KY = KW - K
      CF (K) = RDATA ( KN, KY )
   90 CONTINUE
      CF (3) = CF (3) - CAP
      MOLE = 6RELCAP
      XR = ROOTWO ( KN, 1, CF, MOLE , IW )
      AREA = ( 2.0 * CF (1) * XR ) + CF (2)
      KR = KX - 5
      RESEL = RDATA ( KN, KR ) + XR
      RETURN
      END
      SUBROUTINE PWROPR  (ACFS, JAP, IMON, DAYS, ELEVI, SPILL, IW )

C**** THIS SUBROUTINE SIMULATES THE OPERATION OF A POWEP PLANT WITH ANY
C**** NUMBEP OF UNITS ( GENERATORS ) WHERE EACH AND EVEPY UNIT MUST
C**** HAVE IDENTICAL CAPARILITIES AND CONSTRAINTS . THE ROUTINE AS
C**** DESIGNED ASSUMES UNITS ARF ALWAYS OPERATING AT FULL GATE. HOWEVER,
C**** THE ROUTINE CAN EASILY BE MODIFIED FCR OPFRATION AT BEST GATE OR
C**** A COMBINATION OF BOTH GATE SETTINGS
C**** ALTHOUGH THIS SUBROUTINE SIMULATES ONE UNIT IN A POWEP PLANT ANP
C**** THE NUMBER OF HOURS OF OPERATION ARE IDENTICAL , ** IT IS NOT
C**** NECESSARILY ASSUMED THAT THEY BE THE SAME HOURS IN TIME
      COMMON  / GFNRL / LTITLE(8), NCTRL(20, 3), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMNOD, ISFQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
       COMMON / RFSER / RDATA(20, 110), RULF(20, 13), CONFVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), OINFLO(20, 10, 12), DFMAND(20, 10, 16), K
     BEEMNM(20, 10, 8), KOINNM(20, 10, 8) , KAQUNM (20, 8)
      COMMON  / POWER / CAPBAB(20, 20), TDATA(20, 4), ENERGY(20, 8), PDA
     ATA(20, 12)
      DIMENSION CA (10) , MODE (20)
      DATA  (HPTOKW = 7.457E - 1), (DENS = 6.24E1), (HPF = 5.5E2), (DAF
     A= 4.356E4) , (IFIR = 0 )
C**** CHECK TO DETERMINE IF THIS IS THE FIRST CALL TO THIS SUBROUTINF
C**** FOR THIS JOB
      IF ( IFIR .NE. 0 )  GO TO 20
C**** INITIALIZE CALL INDEX FOR EACH POWEP PLANT
      DO 10 K = 1, 20
      MODE (K) = 0
   10 CONTINUE
      IFIR = 1
   20 KP = JAP
C**** CHECK TO DETERMINE IF THIS IS THE FIRST CALL FOR PARTICULAR POWER
C**** PLANT
      IF ( MODE (KP) . NE. 0 )  GO TO 70
C**** COMPUTE GENFRATOR CAPABILITY ( GENCAP = GENERATOP RATING (KV-A) *
C**** POWER FACTOP * OVERLOAD (PERCENT) / 100.0 ) IN KW
      GENCAP = CAPBAB ( KP, 2) * CAPBAE ( KP, 3) * CAPBAB (4) * 1.0E-2
C**** COMPUTE MAXIMUM HORSEPOWER (HPMAX ) OF TURBINE AS FUNCTION OF
C**** GENERATOR CAPABILITY AND GENERATOR EFFICIENCY
      GENEFF = CAPBAB ( KP, 6 )
      HPMAX = GENCAP * 1.0E2 / ( HPTOKW * GENEFF )
C**** COMPUTE HEAD AT MAXIMUM HORSEPOWER ( THEAD ) AT FULL GATE
C**** USING POLYNOMIAL WHERE HOPSEPOWER IS A FUNCTION OF HEAD **
C**** COEFFICIENTS ARF ARRANGED IN DECREASING POWFRS OF THE
C**** INDEPFNDENT VARIABLE ** POLYNOMIAL IS EITHER SFCOND DEGREE OR
C**** LINFAR
      CA (1) = ENFRGY ( KP,7  )
      CA (2) = ENFRGY ( KP,6  )
      CA (3) = ENFRGY ( KP,5  )
C**** CHECK TO DETEPMINE IF POLYNOMIAL IS LINEAR
      IF ( CA (1) . EQ. 0.0 )  GO TO 30
C**** POLYNOMIAL IS NONLINEAR
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      SUBROUTINE PWROPR  (ACFS, JAP, IMON, DAYS, ELEV1, SPILL, IW )

      MOLE = 6RPWROPR
      THEAD = ROOTWO ( KP, 1 , CA, MOLE, IW )
      GO TO 40
C**** POLYNOMIAL IS LINEAR
   30 THEAD = ( HPMAX - CA(3) ) / CA(2)
C**** COMPUTE MAXIMUM DISCHARGE ( TCFS ) FOR ONE UNIT AT MAXIMUM
C**** HORSEPOWER USING POLYNOMIAL WHERE DISCHARGE IS A FUNCTION OF
C**** HEAD ** POLYNOMIAL HAS SAME CHARACTERISTICS AS THAT FOR
C**** THE COMPUTATION OF HORSEPOWER
   40 DO 50 K = 1, 10
      CA (K) = 0.0
   50 CONTINUE
      DO 60 K = 1, 4
      CA (K) = ENERGY ( KP, K)
   60 CONTINUE
      TCFS = FOFX ( CA , THEAD , 0 )
C**** COMPUTE CONSTANT EFFICIENCY FOR HEADS GREATER THAN HEAD AT
C**** MAXIMUM DISCHARGE
      TEFF = HPMAX * HPF / ( TCFS * THEAD * DENS )
C**** STORE THESE ONE TIME COMPUTED VALUES IN ARRAY CAPBAB
      CAPBAB ( KP,  9 ) = HPMAX
      CAPBAB ( KP, 10 ) = THEAD
      CAPBAB ( KP, 11 ) = TCFS
      CAPBAB ( KP, 12 ) = TEFF
C**** BEGIN SIMULATION  COMPUTATIONS HERE
   70 TEST = ELEV1 - TDATA ( KP, 1 )
      HDMIN = CAPBAB ( KP, 8 )
      HDMAX = CAPBAB ( KP, 7 )
      HPMAX = CAPBAB ( KP, 9 )
      THEAD = CAPBAB (KP, 10 )
      TCFS = CAPBAB ( KP, 11 )
      TEFF = CAPBAB (KP, 12 )
      CONST = DAYS * 2.4E1 * 3.6E3 / DAF
C**** CLEAR VARIABLES CONTAINED IN ARRAY CAPBAB THAT ARE TO BE COMPUTED
C**** DURING THIS CALL
      DO 80 K = 13, 20
      CAPBAB (KP, K ) = 0.0
   80 CONTINUE
      CAPBAB (KP, 16 ) = TDATA ( KP, 1 )
C**** CHECK TO DETERMINE IF RESERVOIR LEVEL IS BELOW MINIMUM POOL IF
C**** SO RETURN WITH POWER = 0
      IF ( TEST . LE. HDMIN )  GO TO 2000
      UNITS = CAPBAB (KP, 1 )
      TSPILL = SPILL / CONST
C**** BEGIN ITERATIVE SCHEME TO COMPUTE POWER ITERATING ON FLOW THROUGH
C**** EACH UNIT*** USE TCFS AS SEED
   90 XT = TCFS * UNITS
      DO 100 K = 1, 4
      CA (K) = TDATA ( KP, K )
      SUBROUTINE PWROPR  (ACFS, JAP, IMON, DAYS, ELEV1, SPILL, IW )

      TWEL = FOFX ( CA, XT , 0 )
C**** COMPUTE GROSS HEAD ( SAME AS NET HEAD SINCE INCIDENTAL HEAD
C**** LOSSES ARE NEGLECTED)** LET KSET BE INDICATOR FOR GHEAD BEING
C**** LESS THAN OR GREATER THAN HEAD AT MAXIMUM HORSE POWER
C**** GROSS HEAD = RESERVOIR WATER SURFACE ELEVATION - TAIL WATER
C**** ELEVATION
      KSET = 0
      GHEAD = ELEV1 - TWEL
      IF ( GHEAD . GT. THEAD )  GO TO 120
C**** GROSS HEAD IS LESS THAN HEAD AT MAXIMUM HORSEPOWER - USING
C**** POLYNOMIAL COMPUTE DISCHARGE AT THIS HEAD
      DO 110 K = 1, 4
      CA (K) = ENERGY ( KP , K )
  110 CONTINUE
      RCFS = FOFX ( CA , GHEAD , 0 )
      GO TO 130
C**** COMPARE GROSS HEAD WITH MAXIMUM HEAD
  120 IF ( GHEAD . GT. HDMAX )  GHEAD = HDMAX
C**** GROSS HEAD IS GREATER THAN HEAD AT MAXIMUM HORSEPOWER
      KSET = 1
      RCFS = ( HPMAX * HPF ) / ( GHEAD * DENS * TEFF )
  130 EPSLON = ABS ( TCFS - RCFS )
      IF ( EPSLON . LT. 5.0 ) GO TO 140
      TCFS = RCFS
      GO TO 90
C**** COMPARE GROSS HEAD TO MINIMUM HEAD
  140 IF ( GHEAD . LT. HDMIN )  GO TO 1000
      IF ( KSET . NE. 0 )  GO TO 160
C**** COMPUTE HORSEPOWER PER UNIT ON BASIS OF GROSS HEAD  ** USING
C**** POLYNOMIAL WHERE HORSEPOWER IS A FUNCTION OF HEAD
      KA = 1
      DO 150 K = 5, 8
      KA = KA + 1
      CA (KA) = ENERGY ( KP, K )
  150 CONTINUE
      THP = FOFX ( CA , GHEAD , 0 )
C**** COMPUTE THEORETICAL HORSEPOWER ASSUMING 100 PERCENT EFFICIENCY
      THEORY = ( RCFS * DENS * GHEAD ) / HPF
C**** COMPUTE EFFICIENCY AS RATIO OF ACTUAL HORSEPOWER TO THEORETICAL
C**** HORSEPOWER
      TEFF = THP / THEORY
      GO TO 170
  160 THP = HPMAX
C**** CONVERT HORSEPOWER TO KILOWATTS
  170 TKW = THP * HPTOKW
C**** COMPUTE TOTAL POWER IN KILOWATTS AND TOTAL DISCHARGE IN CFS FOR
C**** POWER PLANT WHERE EACH UNIT IN PLANT IS ASSUMED IDENTICAL IN EVERY
C**** RESPECT
      TOTKW = TKW * UNITS
      SUBROUTINE PWROPR  (ACFS, JAP, IMON, DAYS, ELEV1, SPILL, IW )

C**** COMPUTE HOURS OF OPERATION PER UNIT AS THE RATIO OF TOTCFS TO
C**** WATER RELEASED FROM RESERVOIR ( ACFS IN ARGUMENT LIST )
      RATIO = ACFS / TOTCFS
      IF ( RATIO . GT. 1.0 ) RATIO = 1.0
      HOURS = RATIO * 2.4E1 * DAYS
C**** COMPUTE POWER IN KILOWATT-HOURS FOR WHOLE POWER PLANT
      KWH = TOTKW * HOURS
C**** COMPUTE TOTAL FLOW THROUGH POWER PLANT IN ACRE FEET
      RELAF = TOTCFS * CONST * DAYS
C**** COMPARE POWER GENERATED WITH POWER REQUIREMENT ( FIRM DEMAND)
C**** FOR THIS TIME FRAME
      RKWH = PDATA ( KP, IMON)
      IF ( KWH . LT. RKWH )  GO TO 1040
C**** POWER GENERATED IS GREATER THAN FIRM REQUIREMENT ** COMPUTE
C***  SECONDARY POWER GENERATED
      KWHSEC = RKWH - KWH
      KWHSEC = KWH - RKWH
C**** SET VARIABLES IN CAPBAB ARRAY
      CAPBAB ( KP, 13 ) = HOURS
      CAPBAB ( KP, 14 ) = KWH
      CAPBAB ( KP, 15 ) = RELAF
      CAPBAB ( KP, 16 ) = TWEL
      CAPBAB ( KP, 17 ) = GHEAD
      CAPBAB ( KP, 18 ) = RKWH
      CAPBAB ( KP, 19 ) = KWHSEC
      CAPBAB ( KP, 20 ) = TEFF
      GO TO 2000
 1000 WRITE ( IW , 1010 )
 1010 FORMAT ( 1H1, 7X, 36HGROSS HEAD IS LESS THAN MINIMUM HEAD )
 1020 KNODE = NCTPL ( KP, 1 )
      WRITE ( IW , 1030 ) KNODE , IMON
 1030 FORMAT ( 8X, 11HFOR NODE =  , I3, 5X, 16HFOR MONTH NO. = , I3 )
      CALL EXIT
 1040 WRITE ( IW , 1050 )
 1050 FORMAT ( 1H1, 7X, 40HPOWER GENERATED IS LESS THAN FIRM DEMAND  )
      GO TO 1020
 2000 RETURN
      END
      SUBROUTINE DTABLE ( JK, KFA, IC, KS )

        COMMON / GENRL / LTITLE(A), NCTRL(20, 3), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMNOD, ISEQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
        COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     BDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,A)
       DIMENSION AREA (20) , KFA (20)
C**** THIS SUBROUTINE SERVES AS A DECISION TABLE TO DETERMINE WHICH OF
C**** THE RESERVOIRS UPSTREAM OF A DEFICIT ( IF ANY) SHOULD BE CALLED
C**** FIRST, SECOND .ETC. BASED UPON THE PREMISE THAT THE RESERVOIR
C**** THAT CAN MAKE A RELEASE WITH THE LEAST LOSS IN ELEVATION ( POWER
C**** HEAD CONCERN ) SHOULD HAVE THE HIGHEST PRIORITY IN THE CALLING
C**** SEQUENCE.  A TABLE SUCH AS THIS OR ANY OTHER CAN AND SHOULD BE AT
C**** THE DESCRETION OF THE ANALYST.  SEARCH THE NODE SEQUENCE ARRAY TO
C**** DETERMINE IF A RESERVOIR EXISTS IN THIS NODE AND IS UPSTREAM OF
C**** DEFICIT
      DO 50 K = 1, KS
      IF ( ISEQ (JK, K ) . EQ. 0 ) GO TO 60
   50 CONTINUE
C**** NO RESERVOIR EXISTS IN NODE OF DEFICIT THAT IS ALSO UPSTREAM OF
C**** DEFICIT
      IC = 0
      GO TO 65
C**** A RESERVOIR EXISTS IN THIS NODE AND SHOULD BE INCLUDED IN RANKING
   60 IC = 1
C**** IN THIS MODEL RESERVOIR CAPACITY = A0 + A1 * H + A2 * H ** 2 ,
C**** THE FIRST DERIVATIVE DC/DH= A1+2*A2*H = RESERVOIR AREA . LET
C**** DC/DH = AREA AND RANK WITH RESPECT TO AREA. AREA = RDATA ( JK, 5 )
C**** IN THE RDATA ARRAY
      AREA (IC ) = RDATA ( JK, 5 )
      KFA ( IC ) = NCTRL ( JK, 1 )
C**** WITH THE USE OF THE ARRAY NDWTR WHICH CONTAINS THE NODE SYSTEM
C**** STRUCTURE SEARCH FOR UPSTREAM RESERVOIRS THAT CAN SERVE THIS NODE
   65 DO 70 K = 1, 20
      IF ( NDWTR ( JK, K) . LE. 0 )  GO TO 80
      NODE = NDWTR ( JK, K)
      KN = NFIND ( NODE )
C**** CHECK TO DETERMINE IF A RESERVOIR EXISTS IN NODE
      IF ( RDATA ( KN, 3 ) . EQ. 0.0 )  GO TO 70
      IC = IC + 1
      AREA (IC ) = RDATA (KN, 5 )
      KFA (IC ) = NDWTR ( JK, K)
   70 CONTINUE
C**** RANK UPSTREAM RESERVOIRS WITH RESPECT TO AREA
   80 MAX = IC
      MIN = 0
   90 MIN = MIN + 1
      IF ( MIN . GE. MAX )  GO TO 2000
      DO 100 K = MIN , MAX
      IF ( AREA (MIN ) . GE. AREA (K) )   GO TO 100
      SUBROUTINE DTABLE ( JK, KFA, IC, KS )

      LTEMP = KFA ( MIN )
      AREA (MIN ) = AREA (K)
      KFA (MIN ) = KFA (K)
      AREA (K) = TEMP
      KFA (K) = LTEMP
  100 CONTINUE
      GO TO 90
 2000 RETURN
      END
      FUNCTION NFIND (NODE)

      COMMON / GENRL / LTITLE(8), NCTRL(20, 3), MOBEG, IYRBEG, MOEND, I
     AYREND, NUMNOD, ISEQ(20, 20), KPRI, NUMSEQ(20), NDWTR(20, 20)
C**** SUBROUTINE FINDS SUBSCRIPT NUMBER FOR NODE PASSED THROUGH ARGUMENT
C**** LIST
      IW = 61
      DO 5 J = 1, NUMNOD
      JK = J
      IF (NODE.EQ.NCTRL(J, 1)) GO TO 10
    5 CONTINUE
      GO TO 15
   10 NFIND = JK
      RETURN
C**** ERROR MESSAGES FOR PROGRAM CONTROLLED ERRORS ARE GENERATED HERE
   15 WRITE (IW, 20) NODE
     XR = 1.0 / 0.0
      CALL EXIT
   20 FORMAT (1H1, 44HNO MATCH WAS FOUND IN CONNOD FOR NODE NUMBER, I5)
     END
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      SUBROUTINE RFCOMP ( QFLOW, NK, IP, INDY, MO, CONST, IW )

        COMMON / PROPER / SOIL(20, 10, 21), BTANK(20, 10), TTANK(20, 10),
     1 GRTANK(20, 10)   , NSEG (20) , CONUSE (20, 10, 30)
     2               , KUSE (20, 10, 30)
        COMMON / RFSER / RDATA(20, 110), RULF(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), KSY
     PDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,8)
       EQUIVALENCE ( CONUSE, KUSE )
       DIMENSION QFLOW (10), RFLOW (10)
C**** THIS SUBROUTINE COMPUTES MAGNITUDE, CHEMISTRY AND THE ALLOCATION
C**** OF RETURN FLOWS. ALSO THE SUBROUTINE COMPUTES SHORTAGES AND
C**** COMPARES THESE WITH THE SHORTAGE INDICES. EXCHANGES BETWEEN
C**** SURFACE FLOWS , SUBSURFACE FLOWS, AND THE SOIL COLUMNS ARE
C**** SIMULATED AS DEMANDS WITHOUT RETURN FLOW ALLOCATIONS.  THERE ARE
C**** ONLY TWO DEMANDS WITH RETURN FLOW ALLOCATIONS AND THOSE ARE FOR
C**** IRRIGATION AND MUNICIPAL AND INDUSTRIAL REQUIREMENTS. DEMANDS
C**** ARE THOSE CONSIDERED IDEAL OR FULL SUPPLY COMPUTED AT THE
C**** POINT OF DIVERSION AND INCLUDE CONVEYANCE LOSSES AND FARM LOSSES
C**** CONSUMPTIVE USE VALUES REPRESENT A LUMPED BENEFICIAL AND NON
C**** BENEFICIAL REQUIREMENT.      QFLOW = VOLUME AND CHEMISTRY OF
C**** SOURCE, NK AND IP ARE THE NODE AND SEQUENCE INDICES RESPECTIVELY
C**** INDY = USE INDEX , MO = MONTH AND IW = WRITE UNIT.
      IF ( INDY .GT. 5 )  GO TO 1010
      GO TO ( 80, 200, 300, 300, 300) , INDY
C**** DEMAND HAS BEEN MET SET SHORTAGE ( PERCENT ) EQUAL TO ZERO
   80 CONUSE ( NK, IP, 15 ) = 0.0
C**** BEGIN TO COMPUTE RETURN FLOW ITS ALLOCATION AND CHEMISTRY
      RFLOW (1) = CONST - CONUSE (NK, IP, MO )
   90 VOLA = CONST
      VOLB = RFLOW (1)
      DO 100 K = 2, 10
      RFLOW (K) = QFLOW (K) * ( VOLA / VOLB )
  100 CONTINUE
      K = 15
  120 K = K + 4
      IF ( K . GT. 27 )  GO TO 2000
      KDES = KUSE ( NK, IP, K)
      KNODE = KUSE (NK, IP, K + 1 )
      IF ( KNODE . LE. 0 )  GO TO 120
      KSEQ = KUSE ( NK, IP, K + 2 )
      KPER = KUSE ( NK, IP, K + 3 )
      JK = NFIND (KNODE )
      PER = KPER
      QINFLO ( JK, KSEQ, 1 ) = RFLOW (1) * PER * 1.0E-2
      DO 130 KA = 2, 10
      QINFLO ( JK, KSEQ, KA ) = RFLOW (KA)
  130 CONTINUE
      IF ( KDES . EQ. 3RSUR ) QINFLO( JK, KSEQ, 11 ) = 1.0
      IF ( KDES . EQ. 3RGWR ) QINFLO( JK, KSEQ, 11 ) = 2.0
      IF ( KDES . EQ. 3RGWV ) QINFLO( JK, KSEQ, 11 ) = 3.0
      SUBROUTINE RFCOMP ( QFLOW, NK, IP, INDY, MO, CONST, IW )

C**** IRRIGATION OR A MUNICIPAL AND INDUSTRIAL USE
      IF ( DEMAND ( NK, IP, 14) . EQ. 1.0 )  KUSE ( NK, IP, 17 ) = 3RIRR
      IF ( DEMAND ( NK, IP, 14) . EQ. 2.0 )  KUSE ( NK, IP, 17 ) = 3RMAI
      GO TO 120
C**** DEMAND HAS NOT BEEN MET COMPUTE SHORTAGE IN PERCENT
  200 RATIO = CONUSE ( NK, IP, 13 ) * 1.0E-2
      TEMCU = CONST * ( 1.0 - RATIO )
      SHORT = ( 1.0 - ( TEMCU / CONUSE (NK, IP, MO))) * 1.0E2
C**** COMPARE SHORTAGE WITH SHORTAGE INDEX
      IF ( SHORT . GT. CONUSE ( NK, IP, 14 )) GO TO 1000
C**** SHORTAGE IS LESS THAN SHORTAGE INDEX COMPUTE RETURN FLOW
      RFLOW (1) = CONST - TEMCU
      CONUSE ( NK, IP, 15) = SHORT
      GO TO 90
C**** WHEN THE INDEX ( INDY ) IS GREATER THAN 2 THE ROUTINE TREATS
C**** THE DEMANDS AS TRANSFERS OF FLOW WITHOUT RETURN FLOW OR
C**** CONSUMPTIVE USE
  300 KDES = KUSE (NK, IP, 19)
      KNODE = KUSE (NK, IP, 20)
      KSEQ = KUSE ( NK, IP, 21 )
      JP = NFIND ( KNODE)
      IF ( CONST . GT. 0.0 )  GO TO 315
      DO 310  K = 1, 10
      QINFLO( JP, KSEQ, K ) = 0.0
  310 CONTINUE
      GO TO 330
  315 QINFLO( JP, KSEQ, 1 ) = CONST
      DO 320 K = 2, 10
      QINFLO ( JP, KSEQ, K ) = QFLOW (K)
  320 CONTINUE
  330 IF ( KDES . EQ. 3RSUR ) QINFLO( JK, KSEQ, 11 ) = 1.0
      IF ( KDES . EQ. 3RGWR ) QINFLO( JK, KSEQ, 11 ) = 2.0
      IF ( KDES . EQ. 3RGWV ) QINFLO( JK, KSEQ, 11 ) = 3.0
      GO TO 2000
 1000 WRITE ( IW, 1005)  (KDEMNM ( NK, IP, K) , K= 1, 8), NK, IP
 1005 FORMAT ( 1H1, 7X, 32HSHORTAGE INDEX IS VIOLATED FOR    , 8A8 /
     1       13HFOR NODE NO.   , I3, 5X, 12HSEGMENT NO.     , I3 )
      CALL EXIT
 1010 WRITE ( IW, 1015 ) INDY , NK, IP
 1015 FORMAT ( 1H1, 7HINDY =   , I3, 5X, 24HWHICH IS GREATER THAN 5  ,
     1       13HFOR NODE NO.   , I3, 5X, 12HSEGMENT NO.   , I3 )
      CALL EXIT
 2000 RETURN
      END
      SUBROUTINE  CHEMGR ( QFLOW , CONST , KN, KS )
        COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     RDEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,8)
        COMMON / PROPER / SOIL(20, 10, 21), RTANK(20, 10), TTANK(20, 10),
     1 GRTANK(20, 10)   , NSEG (20) , CONUSE (20, 10, 30)
     2              , KUSE (20, 10, 30)
       EQUIVALENCE ( CONUSE, KUSE )
       DIMENSION QFLOW (10)
C**** THIS SUBROUTINE IS USED TO COMPUTE A LINEAR MIX OF CHEMISTRY
C**** FOR FLOW ADDED TO THE RIVER ( SURFACE) , TO THE AQUIFER (SUBSURFACE)
C**** , TO THE PONDING POOL ABOVE SOIL COLUMN, AND FLOW ADDED TO THE
C**** RESERVOIR.
C**** QFLOW = FLOW IN RIVER ARRAY . KN AND KS ARE INDICES FOR NODE AND
C**** SEQUENCE RESPECTIVELY, CONST = DEMAND OR DIVERSION
C**** THIS ENTRY MIXES RIVER FLOW WITH AQUIFER
       VOLA = CONST
       VOLB = GRTANK (KN, 1 )
       VOLUME = VOLA + VOLB
       DO 50 K = 2, 10
       GRTANK (KN, K ) = ( QFLOW (K) * VOLA + GRTANK (KN, K ) * VOLB )
     1              / VOLUME
   50 CONTINUE
       GO TO 2000
C**** THIS ENTRY MIXES RIVER FLOW WITH PONDING POOL
       ENTRY CHEMTT
       VOLA = CONST
       VOLB = TTANK (KN, 1 )
       VOLUME = VOLA + VOLB
       DO 60 K = 2, 10
       TTANK (KN, K ) = ( QFLOW (K) * VOLA + TTANK (KN, K ) * VOLB )
     1              / VOLUME
   60 CONTINUE
       GO TO 2000
C*** THIS ENTRY MIXES FLOW TO RIVER WITH RIVER
       ENTRY CHEMRV
       VOLA = QINFLO( KN, KS, 1 )
       VOLB = QFLOW (1)
       VOLUME = VOLA + VOLB
       DO 70 K = 2, 10
       QFLOW (K) =(QINFLO(KN,KS,K) * VOLA + QFLOW (K) * VOLB ) / VOLUME
   70 CONTINUE
       GO TO 2000
C**** THIS ENTRY MIXES RESERVOIR CHEMISTRY WITH RIVER CHEMISTRY FOR
C**** DEFICIT RELEASE
       ENTRY CHEMRS
       VOLA = QFLOW (1)
       VOLB = CONST
       VOLUME = VOLA + VOLB
       DO 90 K = 2, 10
      SUBROUTINE  CHEMGR ( QFLOW , CONST , KN, KS )

      QFLOW (K) = ( QFLOW (K) * VOLA + RDATA ( KN, KA) * VOLB ) / VOLUME
   90 CONTINUE
      GO TO 2000
C**** THIS ENTRY MIXES RIVER FLOW ( AS INFLOW TO RESERVOIR) WITH
C**** RESERVOIR CHEMISTRY
      ENTRY CHEMRR
      VOLA = QFLOW (1)
      VOLB = RDATA ( KN, 3 )
      VOLUME = VOLA + VOLB
      DO 110 K = 2, 9
      KA = K + 99
      RDATA ( KN, KA ) =(QFLOW (K) * VOLA + RDATA ( KN, KA ) * VOLB )
     1            / VOLUME
  110 CONTINUE
      GO TO 2000
C**** THIS ENTRY MIXES AQUIFER FLOW WITH RIVER FLOW
      ENTRY CHEMAQ
      VOLA = QFLOW (1)
      VOLB = GRTANK (KN, 1 )
      VOLUME = VOLA + VOLB
      DO 130 K = 2, 9
      QFLOW (K) = ( QFLOW (K) * VOLA + GRTANK ( KN, K ) * VOLB)/ VOLUME
  130 CONTINUE
      GO TO 2000
C**** THIS ENTRY MIXES BTANK WATER WITH AQUIFER
      ENTRY CHEMBT
      VOLA = QFLOW (1)
      VOLB = GRTANK (KN, 1)
      VOLUME = VOLA + VOLB
      DO 140 K = 2, 10
      GRTANK (KN, K) = ( QFLOW (K) * VOLA + GRTANK (KN,K) * VOLB ) /
     1            VOLUME
  140 CONTINUE
      GRTANK (KN, 1 ) = VOLUME
 2000 RETURN
      END
      SUBROUTINE CONVER ( TEMP , KR )
C**** THIS SUBROUTINE IS USED TO CONVERT INPUT UNITS TO PPM AND
C**** ALSO TO CHECK BALANCE BETWEEN CATIONS AND ANIONS
      DIMENSION TEMP (15) , EQVWT (8)
      DATA ((EQVWT(K), K=1,8) = 20.04,12.16,23.,35.46,48.03,30.,61.01,
     1                          62.008 )
      IF ( KR . NE. 1 )  GO TO 80
C**** UNITS ARE IN MILLIEQUIVALENTS PER LITER  CHECK SUM OF CATIONS
C**** AND ANIONS
C**** SUM CATIONS
   10 SUMC = 0.0
      DO 20 K = 2, 4
      SUMC = SUMC + TEMP (K)
   20 CONTINUE
C**** SUM ANIONS
      SUMA = 0.0
      DO 30 K = 5,9
      SUMA = SUMA + TEMP (K)
   30 CONTINUE
      DIFF = SUMC - SUMA
      IF ( DIFF . GT. 0.0 )   GO TO 40
      TEMP (2) = TEMP (2) + ABS ( DIFF )
      GO TO 45
   40 TEMP (6) = TEMP(6) + DIFF
C**** CONVERT FROM MILLIEQUIVALENTS PER LITER TO PARTS PER MILLION
   45 DO 50 K = 2, 9
      KA = K - 1
      TEMP (K) = TEMP (K) * EQVWT ( KA )
   50 CONTINUE
C**** COMPUTE TOTAL DISSOLVED SOLIDS FROM ANALYSIS
      TDS = 0.0
      DO 70 K = 2, 9
      IF ( K . EQ. 7 )  GO TO 60
      TDS = TDS + TEMP (K)
      GO TO 70
   60 TDS = TDS + ( TEMP (K) * 5.0E-1 )
   70 CONTINUE
      TEMP (10 ) = TDS
      WRITE ( 61, 75) ( TEMP (K) , K = 1, 10 )
   75 FORMAT ( 8X, 10 ( 2X, F10.2 ))
      GO TO 2000
C**** CONVERT PARTS PER MILLION TO MILLIEQUIVALENTS PER LITER
   80 DO 85 K = 2, 9
      KA = K- 1
      TEMP (K) = TEMP (K) / EQVWT (KA)
   85 CONTINUE
      GO TO 10
 2000 RETURN
      END
      SUBROUTINE VERNAL ( KN, IS, MO, OBSERV , QFLOW )

C**** THIS SUBROUTINE SIMULATES THE ASSUMED CRITERIA FOR EACH NODE
C**** IN OBTAINING A HYDROLOGIC BALANCE WITH SIMPLE TRANSFERS FROM
C**** SURFACE TO SUBSURFACE OR THE CONVERSE. THE ARGUMENT LIST IS
C**** AS FOLLOWS - KN AND IS ARE THE NODE AND SEQUENCE INDICES
C**** RESPECTIVELY. OBSEVR IS THE ARRAY CONTAINING THE OBSERVED OUTFLOWS
C**** QFLOW IS THE ARRAY CONTAINING THE RIVER VOLUME AND CHEMISTRY
       COMMON / RESER / RDATA(20, 110), RULE(20, 13), CONEVP(20, 12), BA
     ANKCO(20), KSURNM(20, 8), QINFLO(20, 10, 12), DEMAND(20, 10, 16), K
     *DEMNM(20, 10, 8), KQINNM(20, 10, 8) , KAQUNM (20,8)
      DIMENSION OBSERV (10) , QFLOW (10)
      GO TO ( 50, 70, 90 ) , KN
C**** THESE ARE THE TRANSFER PARAMETERS FOR NODE 101
   50 MIN = 3
      MAX = 7
      KA = 4
      GO TO 110
C**** THESE ARE THE TRANSFER PARAMETERS FOR NODE 102
   70 MIN = 2
      MAX = 6
      KA = 3
      GO TO 110
C**** THESE ARE THE TRANSFER PARAMETERS FOR NODE 103
   90 MIN = 2
      MAX = 4
      KA = 3
  110 IF ( IS .GT. MIN )   GO TO 150
      DO 130 K = 1, 10
      OBSERV (K) = QINFLO ( KN, IS, K)
  130 CONTINUE
      GO TO 2000
  150 VOLA = OBSERV (1)
      VOLB = QINFLO (KN, IS, 1)
      VOLUME = VOLA + VOLB
      DO 170 K = 2, 10
      OBSERV (K) = ( OBSERV (K) * VOLA + QINFLO (KN, IS, K ) * VOLB ) /
     1         VOLUME
  170 CONTINUE
      OBSERV (1) = VOLUME
      IF ( IS.LT. MAX )   GO TO 2000
      KB = KA - 1
      DIFF = OBSERV (1) - QFLOW (1)
      IF ( DIFF . LT. 0.0 ) GO TO 190
C**** VOLUME OF OBSERVED OUTFLOW IS GREATER THAN THE PREDICTED OUTFLOW
C**** SET UP TRANSFER OF RIVER FLOW TO THE AQUIFER
      DEMAND ( KN, KA, MO ) = DIFF
      DEMAND ( KN, KB, MO ) = 0.0
      GO TO 2000
C**** VOLUME OF OBSERVED OUTFLOW IS LESS THAN THE PREDICTED OUTFLOW
C**** SET UP TRANSFER FROM THE AQUIFER TO THE RIVER
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      SUBROUTINE VERNAL ( KN, IS, MO, OBSERV , QFLOW )

      DEMAND (KN, KB, MO ) = ABS (DIFF)
 2000 RETURN
      END
      FUNCTION ROOTWO ( KNODE , KSEG , CA , MOLE , IW )
C
CALCULATE ROOT OF (X) USING QUADRATIC WHERE
C**** X = ( - B + SQRT ( B*B - 4 * A * C ) / 2 A     KNODE = NODE
C**** INDEX AND KSEG = SEGMENT INDEX  CA = ARRAY OF COEFFICIENTS
C**** IN DECREASING POWERS OF (X)   MOLE = ALPHA DEFINITION OF (X)
      DIMENSION CA (10)
      RAD = CA (2) * CA (2) - ( 4.0 * CA (1) * CA (3) )
      IF ( RAD . LE. 0.0 ) GO TO 1000
      ROOTWO = ( - CA (2) + SQRT ( RAD )) /(2.0 * CA (1))
C  40 WRITE ( IW , 50 ) MOLE , CA(1) , CA(2) , CA(3) , RAD , ROOTWO
C  50 FORMAT ( 1H1, 8X, R6, 2X,
C    1           9HCA (1) = , F15.8, 2X,
C    1           9HCA (2) = , F15.8, 2X,
C    1           9HCA (3) = , F15.8, 2X,
C    1           9HRADCAL = , F15.8 / 9X,
C    1           9HROOTWO = , F15.8 )
      GO TO 2000
 1000 WRITE ( IW , 1005 ) KNODE , KSEG , MOLE
 1005 FORMAT(1H1, 8X, 25HPROBABLY NOT A REAL ROOT  , 5X, 11HSET ROOT TO
     1      5H ZERO  , 5X, 7HNODE =  , I3 , 5X, 6HSEG =  , I3, 5X,
     2      4HFOR   , R6, 2X, 11HCOMPUTATION  )
 2000 RETURN
      END
      FUNCTION ROOT (CONST, XMAX, XMIN , MOLE , CA, TESTA )

C**** THIS FUNCTION WILL COMPUTF THE REAL ROOT IF ONE EXISTS
C**** IN THE RANGF XMIN - XMAX INCLUSIVE. IF A ROOT EXISTS IN THIS RANGE
C**** MOLE WILL BF SET = TRUE. IF NO ROOT EXISTS , MOLE WILL BE SET =
C**** FALSE. F (X) = CONST AND COEFFICIENTS CA (1) )) CA (N+1 ) ARE
C**** TRANSFERRED THROUGH ARGUMENT LIST IN INCREASING POWERS OF THE
C**** INDEPENDENT VARIABLE.  IN THE FUNCTION FOFX NK = 5 , SO IF  A
C**** A HIGHER THAN FOURTH DEGREE POLYNOMIAL IS TO SOLVFD RESET NK .
C**** IF NO ROOT IS FOUND AFTER TWENTY ITERATIONS NO ROOT WILL BE
C**** CONSIDERED AND MOLE WILL BE SET = NONE.
      DIMENSION  CA(10)
      XA = 1.E-1 * XMAX
      IF ( XMIN . LT. 0.0 ) XA = 1.E-1 * XMIN
      XB = XA + XA
      IW = 61
C     WRITE ( IW , 5 ) XMAX , XMIN , MOLE
C   5 FORMAT ( 1H1, 8X, 7HXMAX =    , F15.8, 5X, 7HXMIN = , F15.8 , 5X,
C    1         4HFOR    , R6 // )
      DO 15 K= 1, 5
C     WRITE ( IW , 10 )  K , CA (K)
C  10 FORMAT ( 8X, 4HCA(    , I2 , 5H ) = , F20.8 // )
   15 CONTINUE
C     WRITE ( IW , 18 )
C  18 FORMAT ( 10X, 2HXA , 18X, 3HFXA , 18X, 2HXB , 18X, 3HFXB , 18X,
C    1            2HXC , 16X, 5HCONST  / )
      MOLE = 5RTRUE
      NK = 0
      CA(1) = CA(1) - CONST
      FXA = FOFX ( CA , XA, 1 )
      GO TO 30
   20 FXA = FXB
   30 NK = NK + 1
      IF(NK.GT.20)  GO TO 100
      FXB = FOFX ( CA, XB, 1 )
      DX = XB - XA
      DXDP = FXB - FXA
      IF(DXDP.EQ.0.0)  GO TO 50
      XC = XB - DX * FXB / DXDP
C     WRITE(61,  40) XA, FXA, XB, FXB, XC, CONST
C  40 FORMAT (  6F20.10  )
      EPSLON =  ABS (XC - XB)
      IF ( ABS (EPSLON) . LT.TESTA  )  GO TO 50
      XA = XB
      XB = XC
      GO TO 20
   50 ROOT = XB
      IF(XB.GT.XMAX.OR.XB.LT.XMIN) MOLE = 5RFALSE
      GO TO 2000
  100 ROOT = 0.0
      MOLE = 5RNONE
```

```
FUNCTION ROOT (CONST, XMAX, XMIN , MCLE , CA, TESTA )
END
```

```
      FUNCTION FOFX(CF,X, KAM )
C****
C**** THIS FUNCTION EVALUATES ANY POLYNOMIAL  FROM 1ST DEGREE TO
C**** FOURTH DEGREE INCLUSIVE ( SEE SETTING OF NK ) IF A HIGHER DEGREE
C**** POLYNOMIAL IS TO BE EVALUATED RESET NK  WHERE NK - 1 = DEGREE
      DIMENSION  CF(10)
      FOFX = 0.0
      NK = 5
   30 FOFX = FOFX + CF(NK)
      FOFX = FOFX * X
      NK = NK - 1
      IF(NK.GT.1)  GO TO 30
      FOFX = FOFX + CF(1)
      IF ( KAM . NE. 0 ) GO TO 2000
      DO 40 K = 1, 10
      CF (K) = 0.0
   40 CONTINUE
 2000 RETURN
      END
      SUBROUTINE SOILCO ( KNODE , IW , IR , NSEGS)
C****
C**** THIS SUBROUTINE IS USED AS A MONITOR SUBROUTINE FOR ALL SUB-
C**** ROUTINES USED IN THE SIMULATION OF PERCOLATING APPLIED WATERS
C**** VERTICALLY THROUGH A SOIL COLUMN USING PISTON DISPLACEMENT OF
C**** SOLUTION FROM SEGMENT TO SEGMENT. THE FIRST STEP IS TO CHECK
C**** FOR FIRST CALL TO THIS SUBROUTINE -- IF FIRST CALL CLEAR ARRAY
C**** ITER WHERE TALLY IS KEPT FOR NUMBER OF TIMES SEGMENT HAS BEEN
C**** EQUILIBRATED FOR EACH APPLICATION OF WATERS TO BE PERCOLATED
C**** AND ALSO ARRAY KWATER WHERE TALLY IS KEPT OF EACH APPLICATION
C**** OF NEW WATER.
      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                  SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLTD/ CATEX, GYPSUM, SLIME ,BDENS, EXCA ,EXNA, EXMG ,
     1                EXTRAC , DEPTH, SEGVOL , INTER
      DIMENSION ITER (20, 10 ) , KWATER (20) , CA (10)
      DATA ( IFIR = 0 )
      IF ( IFIR .NE. 0 ) GO TO 25
      DO 20 K = 1, 20
      KWATER (K) = 0
   20 CONTINUE
      IFIR = 1
   25 DO 30 I = 1, 20
      DO 30 J = 1, 10
      ITER ( I, J) = 0
   30 CONTINUE
      IF ( KWATER (KNODE ) . GT. 0 )  GO TO 300
      ISW = 0
      MAX = NSEGS
      MIN = 1
C**** BEGIN EQUILIBRATION OF ALL SEGMENTS IN SOIL COLUMN FOR A
C**** A PARTICULAR ITERATION INDEX
   35 DO 200 K = MIN , MAX
      NCT = 0
C**** UPDATE COUNTER (ITER) WHICH INDICATES NUMBER OF TIMES THE
C**** KTH SEGMENT HAS BEEN EQUILIBRATED
      ITER (KNODE , K ) = ITER ( KNODE , K ) + 1
C**** PLACE DATA FROM SOIL ARRAY INTO COMPUTATIONAL VARIABLE
C**** NAME SEQUENCE FOR THE KTH SEGMENT
      CALL SETUP ( KNODE , K , NSEGS, ISW )
C     WRITE ( IW , 40) ITER ( KNODE , K ) , KNODE , K
C  40 FORMAT ( 1H1, 7X,41HBEGINNING CONDITIONS-EQUILIBRATION NO. = ,I2/
C    1                8X, 11HFOR NODE = , I3, 5X,10HSEGMENT =  , I2/ )
C     CALL SCRIBE (IW)
CALCULATE MOISTURE CONTENT (WRATIO) = GRAMS OF WATER / GRAMS OF SOIL
C**** FOR THE INITIAL SOIL ANALYSIS WRATIO = EXTRACT (EXTRAC) . MOISTURE
C**** CONTENT FOR APPLIED WATERS IS A FUNCTION OF VOLUME OF WATER,
C**** BULK DENSITY AND DEPTH OF KTH SEGMENT
C**** MOISTURE CONTENT IN PERCENT (PRATIO) = WRATIO * 1.E2
      WRATIO = EXTRAC
      SUBROUTINE SOILCO ( KNODE , IW , IR , NSEGS)

      PRATIO = WRATIO * 1.E2
      IF ( KWATER (KNODE ) . GT. 0 )  GO TO 50
C**** IF APPLIED WATERS HAVE NOT BEEN PERCOLATED THROUGH SOIL
C**** COLUMN - EQUILIBRATE ON BASIS OF ORIGINAL SOIL ANALYSIS
CALL SUBROUTINE TO EQUILIBRATE INITIAL SOIL ANALYSIS FOR EACH SEGMENT
      CALL FRSTIM ( KNODE , K, IW )
C     CALL SCRIBE (IW)
CALL SUBROUTINE TO CALCULATE SOLUTION - PRECIPITATION OF GYPSUM **
CASO4 . 2H2O
   50 CALL GYPEX   ( KNODE , K, IW , PRATIO )
C     CALL SCRIBE (IW)
C     CALL SCRIBE (IW)
      CA (1) = SLCA
CALL SUBROUTINE TO CALCULATE EXCHANGE OF CALCIUM AND SODIUM
      CALL EXCANA  ( KNODE , K, IW , PRATIO )
C     CALL SCRIBE (IW)
      CA (2) = SLCA
CALL SUBROUTINE TO CALCULATE EXCHANGE OF CALCIUM AND MAGNESIUM
      CALL EXCAMG  ( KNODE , K, IW , PRATIO )
C     CALL SCRIBE (IW)
      CA (3) = SLCA
CALL SUBROUTINE TO CALCULATE REACTION OF CALCIUM WITH CARBONATE -
C**** BICARBONATE SYSTEM
      CALL CALCAR  ( KNODE , K, IW , PRATIO )
C     CALL SCRIBE (IW)
      CA (4) = SLCA
CHECK TO DETERMINE IF EQUILIBRIUM HAS BEEN ATTAINED IN THE SOIL - WATER
C**** SYSTEM USING CONCENTRATION OF CALCIUM IN SOLUTION AS THE
CONVERGENT VARIABLE
C     WRITE ( IW, 60 ) NCT , ( CA (M) , M = 1, 4 )
C  60 FORMAT ( 1H1, 8X, 10HCOUNTER =  , I2 , / 4 ( 8X, F15.8 ))
      NCT = NCT + 1
      IF ( NCT , GT. 10 )  GO TO 200
      DO 70 L = 1, 4
      EPSLON = CA (L) - SLCA
      IF ( ABS (EPSLON) . GT. 5.E-4 )  GO TO 50
   70 CONTINUE
C**** KTH SEGMENT HAS BEEN EQUILIBRATED CALL SUBROUTINE ENTRY TO LOAD
C**** COMPUTATIONAL SEQUENCE BACK INTO SOIL ARRAY
      CALL RELOAD ( KNODE , K , NSEGS , IW )
C     WRITE ( IW , 80 ) NCT, (CA (M) , M = 1, 4 )
C  80 FORMAT ( // 8X, 10HCOUNTER =  , I2   / 4 ( 8X, F15.8) /
C    1                 17HENDING CONDITIONS / )
C     CALL SCRIBE (IW)
  200 CONTINUE
C**** THE SOIL COLUMN HAS BEEN EQUILIBRATED FOR THIS PARTICULAR
C**** ITERATION ** TEST FIRST TO DETERMINE IF THIS ITERATION WAS FOR
C**** THE EQUILIBRATION OF THE ORIGINAL SOIL ANALYSIS
      IF ( KWATER ( KNODE ) . EQ. 0 )   GO TO 300
      SUBROUTINE SOILCO ( KNODE , IW , IR , NSEGS)
C**** OF SURFACE WATERS
      GO TO 310
C**** MOVE APPLIED WATER INTO FIRST SEGMENT AND  EQUILIBRATE
  300 MIN = 0
      MAX = NSEGS
C**** UPDATE COUNTER OF NUMBER OF APPLICATIONS OF SURFACE WATERS
      KWATER ( KNODE ) = KWATER (KNODE ) + 1
      ISW = 3
  310 MIN = MIN + 1
      IF ( MIN . GT. NSEGS )  GO TO 350
      KV = MIN
      CALL SMOVER ( KNODE , KV , NSEGS , ISW )
      GO TO 35
C**** THIS IS THE LAST EQUILIBRATION FOR THIS SOIL COLUMN FOR THIS TIME
C**** FRAME ** MIX SOLUTION IN LOWEREMOST SEGMENT WITH BTANK **** SET
C**** VOLUME OF BTANK
  350 ISW = 4
      CALL SMOVER ( KNODE , KV , NSEGS , ISW )
      GO TO 2000
 2000 RETURN
      END
      SUBROUTINE SETUP ( KN , KV, NSEGS, ISW )

C**** THIS SUBROUTINE HAS MULTIPLE ENTRIES AND CONTROLS THE TRANSFER
C**** OF DATA TO AND FROM THE COMPUTATIONAL VARIABLE NAME SEQUENCE AS
C**** THIS DATA RELATES TO THAT STORED IN THE ARRAY TITLED SOIL. THE
C**** SUBROUTINE ALSO SIMULATES THE VERTICAL DISPLACEMENT OF SOLUTION
C**** FROM ONE SEGMENT TO THE NEXT LOWER SEGMENT (PISTON EFFECT). KN AND
C**** KV IN THE ARGUMENT LIST REPRESENT THE NODE INDEX AND SEGMENT INDEX
C**** RESPECTIVELY.
      COMMON/PROPER / SOIL(20,10,21), ETANK (20,10), TTANK (20,10),
     1                GRTANK (20,10)
      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLID/ CATEX, GYPSUM, SLIME ,BDENS, EXCA ,EXNA, EXMG ,
     1               EXTRAC , DEPTH, SEGVOL , INTER
      DATA ((EQVWT(K), K=1,8) = 20.4 ,12.16,23.,35.46,48.03,30.,61.01,
     1                         62.008 )
      DIMENSION  EQVWT (8) , VALNCE (8)
      REAL INTER
      DATA ((VALNCE (K), K =1,8) = 2., 2., 1.,1.,2.,1.,2.,1.)
C**** THE MAIN ENTRY TO THIS SUBROUTINE CONVERTS UNITS OF INITIAL SOIL
C**** ANALYIS INTO COMPUTATIONAL UNITS
CONVERSION OF MILLIEQUIVALENTS PER LITER (MEQ/L) TC COMPUTATIONAL UNITS
C**** OF MOLS PER LITER (SOLUTION)- MOLS/LITER =(MEQ/L) /(VALENCE * 1.E3)
      IF ( ISW . NE. 0 ) GO TO 70
   50 DO 60 K = 1,8
      SOIL (KN,KV,K) = SOIL (KN,KV,K) / (VALNCE (K) * 1.E3)
   60 CONTINUE
CONVERT MILLIEQUIVALENTS PER 100 GRAMS TO COMPUTATION UNITS OF MOLS/GRAM
C**** WHEN ISW = 0 CONVERSION IS NECESSARY FOR INITIAL SOIL ANALYSIS
C**** PER GRAM (SOLID)- MOLS/GRAM = (MEQ/100GRAMS) /(VALENCE * 1.E5)
      SOIL (KN,KV,11) = SOIL (KN,KV,11)/ (VALNCE(4)* 1.E5)
      SOIL (KN,KV,12) = SOIL (KN,KV,12)/ (VALNCE(5)* 1.E5)
C**** WHEN ISW NOT EQUAL ZERO COMPUTATIONAL UNITS RETAINED NO
C**** CONVERSION REQUIRED
C**** PLACE DATA OF SOIL ARRAY IN COMPLTATIONAL VARIABLE NAME SEQUENCE
   70 SLCA   = SOIL (KN,KV, 1)
      SLMG   = SOIL (KN,KV, 2)
      SLNA   = SOIL (KN,KV, 3)
      SLCL   = SOIL (KN,KV, 4)
      SLSO4  = SOIL (KN,KV, 5)
      SLHCO3 = SOIL (KN,KV, 6)
      SLCO3  = SOIL (KN,KV, 7)
      SLNO3  = SOIL (KN,KV, 8)
      EXTRAC = SOIL (KN,KV, 9)
      SEGVOL = SOIL (KN,KV,10)
      CATEX  = SOIL (KN,KV,11)
      GYPSUM = SOIL (KN,KV,12)
      SLIME  = SOIL (KN,KV,13)
      BDENS  = SOIL (KN,KV,14)
      DEPTH  = SOIL (KN,KV,15)
      SUBROUTINE SETUP ( KN , KV, NSEGS, ISW )

      EXMG   = SOIL (KN,KV,17)
      EXNA   = SOIL (KN,KV,18)
      UCASO4 = SOIL (KN,KV,19)
      UMGSO4 = SOIL (KN,KV,20)
      INTER  = SOIL (KN,KV,21)
      GO TO 2000
C**** THIS ENTRY MOVES OF SOLUTION OF BOTTOMMOST SEGMENT INTO BTANK ARRAY
C**** USING A LINEAR MIX AFTER CONVERTING UNITS OF COMPUTATIONAL MODE TO
C**** PARTS PER MILLION(PPM)  WHERE PPM = MOLES PER LITER * EQUIVALENT
C**** WEIGHT OF SPECIES * VALENCE OF SPECIES * 1.E3 . ALSO MOVES SOLUTION
C**** OF ONE SEGMENT TO NEXT LOWER SEGMENT KEEPING COMPUTATIONAL UNITS OF
C**** MOLES PER LITER  AS WELL AS PLACING APPLIED WATERS IN SOLUTION OF
C**** UPPERMOST SEGMENT CONVERTING UNITS OF PPM  TO MOLS/LITER  WHERE
C**** MOLS PER LITER = PPM /(EQUIVALENT WEIGHT * VALENCE * 1.E3)
      ENTRY SMOVER
      KG = KV
      IF ( KV . GT. 1 ) KG = KV - 1
      KR = NSEGS
      DO 90 K =1,8
      L = K + 1
      BTANK (KN,L) =(BTANK (KN,L) +(SOIL (KN,KR,K)* EQVWT(K) * VALNCE(K)
     1              * 1.E3 )) * 5.E-1
   90 CONTINUE
      IF ( ISW . EQ. 4 ) GO TO 2000
C**** MOVE SOLUTION OF ONE SEGMENT TO NEXT LOWER SEGMENT
   95 KR = KR - 1
      IF ( KR . LT. KG )  GO TO 120
   97 KP = KR + 1
      DO 100 K = 1, 8
      SOIL(KN,KP,K) = SOIL(KN,KR,K)
  100 CONTINUE
      SOIL (KN,KP,19) = SOIL(KN,KR,19)
      SOIL (KN,KP,20) = SOIL(KN,KR,20)
      GO TO 95
  120 IF ( KV. GT. 1 )  GO TO 2000
C**** PLACE APPLIED WATERS INTO UPPERMOIST SEGMENT
      DO 130 K = 1, 8
      L = K + 1
      SOIL(KN, 1,K) = TTANK(KN,L) / (EQVWT(K) * VALNCE(K) * 1.E3)
  130 CONTINUE
      GO TO 2000
C**** AT THE COMPLETION OF EQILIBRATION OF EACH SEGMENT THIS ENTRY RELOADS
C**** ARRAY SOIL BY TRANSFER OF DATA FROM COMPUTATIONAL VARIABLE NAME
C**** SEQUENCE.  ALL UNITS ARE IN COMPUTATIONAL UNITS.
      ENTRY RELOAD
      SOIL (KN,KV, 1) = SLCA
      SOIL (KN,KV, 2) = SLMG
      SOIL (KN,KV, 3) = SLNA
      SOIL (KN,KV, 4) = SLCL
      SUBROUTINE SETUP ( KN . KV. NSEGS. ISW )

      SOIL (KN.KV. 6) = SLHCO3
      SOIL (KN.KV. 7) = SLCO3
      SOIL (KN.KV. 8) = SLNO3
      SOIL (KN.KV.12) = GYPSUM
      SOIL (KN.KV.13) = SLIME
      SOIL (KN.KV.16) = EXCA
      SOIL (KN.KV.17) = FXMG
      SOIL (KN.KV.18) = EXNA
      SOIL (KN,KV,19) = UCASO4
      SOIL (KN.KV.20) = UMGSO4
      SOIL (KN.KV.21) = INTER
 2000 RETURN
      END
      SUBROUTINE FRSTIM ( KNODE , KSEG , IW )
C**** THIS SUBROUTINE IS USED TO CALCULATE IONIC CONCENTRATIONS
C**** OF CALCIUM, MAGNESIUM ,SULFATE AND THE UNDISSOCIATED CALCIUM
C**** SULFATE AND MAGNESIUM SULFATE . THE SUBROUTINE ALSO CALCULATES
C**** THE EXCHANGEABLE CALCIUM ,MAGNESIUM AND SODIUM . THIS SUBROUTINE
C**** IS USED ONLY ONCE FOR EACH SOIL SEGMENT AND USES DATA FROM INITIAL
C**** SOIL ANALSIS.
      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                 SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLID/ CATEX, GYPSUM, SLIME ,BDENS, EXCA ,EXNA, EXMG ,
     1               EXTRAC , DEPTH, SEGVOL , INTER
      DIMENSION CA(10)
      DATA (TECA= 4.9E-3),(TECMG= 5.9E-3)
CALCULATE ACTIVITY COEFFICIENT FOR DIVALENT ION (GAMMA2)
      GAMMA2 = GAMMA (2)
CALCULATE CONCENTRATION OF UNCOMBINED SULFATE ION AS A POSITIVE REAL
C**** ROOT OF A THIRD DEGREE POLNOMIAL . LET THERMODYNAMIC EQUILIBRIUM
C**** CONSTANTS FOR UNDISSOCIATED CALCIUM SULFATE AND MAGNESIUM SULFATE
C**** = 4.9E-3 AND 5.9E-3 RESPECTIVELY
CHECK FIRST TO DETERMINE IF SULFATE IS IN SOLUTION - IF NO SULFATE IS
C**** SOLUTION BYPASS COMPUTATIONS WHERE SULFATE IS A VARIABLE
      IF(SLSO4.LE.0.0)  GO TO 60
CALCULATE COEFFICIENTS FOR THIRD DEGREE POLYNOMIAL
      DO 50 K = 1,10
      CA(K) = 0.0
   50 CONTINUE
      GSQR = GAMMA2 * GAMMA2
      CA(4) = GSQR * GSQR
      CA(3) = GSQR *(TECA + TECMG) + GSQR * GSQR * (SLCA + SLMG -SLSO4)
      CA(2) =  TECA* TECMG + GSQR *(TECMG* SLCA + TECA* SLMG - SLSO4 *
     1        (TECA + TECMG))
      CA(1) = - SLSO4 * TECA * TECMG
C**** CALCULATE UNCOMBINED SO4 AS ROOT GREATER THAN ZERO AND LESS THAN
C**** SLSO4
      CONST = 0.0
CALCULATE A POSITIVE ROOT (REAL) IN RANGE XMIN - XMAX
      XMIN = 0.0
      XMAX = SLSO4
C**** SET CONVERGENCE CRITERION (TESTA) SO THAT F(X) IS LESS THAN 1.E-6
      TESTA = 1.E-6
      MOLE = 6RFRSTIM
      FSO4 = ROOT (CONST,XMAX, XMIN, MOLE , CA , TESTA )
      IF(MOLE.NE.5RTRUE ) GO TO 900
CALCULATE CONCENTRATION OF UNDISSOCIATED CASO4 (MOLS/LITER)
      UCASO4 = SLCA * FSO4 * GSQR / (TECA + GSQR * FSO4)
CALCULATE UNCOMBINED CA (MOLES/ LITER)
      SLCA = SLCA - UCASO4
CALCULATE CONCENTRATION OF UNDISSOCIATED MGSO4 (MOLS/ LITER)
      UMGSO4 =  SLMG * FSO4 * GSQR / (TECMG + GSQR * FSO4)
CALCULATE UNCOMBINED MG (MOLS / LITER)
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      SUBROUTINE FRSTIM ( KNODE , KSEG , IW )

C**** CHANGE CONCENTRATIONS OF DIVALENT IONS FROM MOLS PER LITER TO
C**** EQUIVALENTS PER LITER
      SLMG = SLMG * 2.
      SLCA = SLCA * 2.
      GO TO 70
   60 FSO4 = 0.0
CALCULATE EXCHANGEABLE CALCIUM (EXCA) IN EQUIVALENTS PER GRAM
C**** LET E[illegible]HANGE CONSTANT CA-MG = 0.67 AND FOR CA-NA = 2.0
CALCULATE ACTIVITY COEFFICIENT FOR MONOVALENT ION (GAMMA1)
   70 GAMMA1 = GAMMA (1)
      EXCA =  SLNA * GAMMA1/(2.0 * SQRT(SLCA * GAMMA2))  + 1.0  + 6.7E-1
     1          * SLMG /SLCA
      EXCA = CATEX / EXCA
CALCULATE EXCHANGEABLE SODIUM  (EXNA) IN EQUIVALENTS PER GRAM
      EXNA = EXCA * SLNA * GAMMA1 / (2.0 * SQRT (SLCA * GAMMA2))
CALCULATE EXCHANGEABLE MAGNESIUM (EXMG) IN EQUIVALENTS PER GRAM
      EXMG = CATEX - EXCA - EXNA
C**** CHANGE UNITS FROM EQUIVALENTS PER GRAM AND EQUIVALENTS PER
C**** LITER TO MOLS PER GRAM AND MOLS PER LITER
      EXCA = EXCA * 5.E-1
      EXMG = EXMG * 5.E-1
      SLMG = SLMG * 5.E-1
      SLCA = SLCA * 5.E-1
      SLSO4 = FSO4
      GO TO 2000
C**** ERROR MESSAGES ARE PRINTED HERE
  900 WRITE (IW,910) KNODE , KSEG
  910 FORMAT (1H1,14HERROR IN NODE  ,I3 ,2X ,12HSEGMENT NO. , I3,
     1          15HBECAUSE OF ****    )
  960 WRITE (IW,965) FSO4 , SLSO4
  965 FORMAT (8X , 20HROOT IS OUT OF RANGE , 7HROOT =   ,F10.5 ,
     1         8X,15HRANGE = 0.0 TO  , F10.5  )
      CALL EXIT
 2000 RETURN
      END
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      SUBROUTINE GYPEX (KNODE, KSEG, IW, PRATIO )

C**** THIS SUBROUTINE IS USED TO CALCULATE THE SOLUTION OR PRECIPITATION
C**** OF GYPSUM ( CASO4*2H2O ) AND THE REQUIREMENTS OF CALCIUM
C**** AND MAGNESIUM FOR THE UNDISSOCIATED ION PAIRS CASO4 AND MGSO4.
      DIMENSION CA (10)
      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                 SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLID/ CATEX, GYPSUM, SLIME ,BDENS, EXCA ,EXNA, EXMG ,
     1               EXTRAC , DEPTH, SEGVOL , INTER
CALCULATE ACTIVITY COEFFICIENCT OF DIVALENT ION (GAMMA2)
      GAMMA2 = GAMMA (2)
      GSQR = GAMMA2 * GAMMA2
CALCULATE CHANGES IN CONCENTRATIONS OF CALCIUM AND SULFATE (X). GIVEN THE
C**** SOLUBILITY PRODUCT (KSP) OF GYPSUM = 2.4E-5. SOLVE FOR (X) USING
C**** QUADRATIC  FORM OF KSP = ((SLCA + X)(SLSO4 +X))* GAMMA2 **2 . WHEN
C**** (X) IS POSITIVE SOLUTION IS UNDERSATURATED. WHEN (X) IS ZERO OR
C**** NEGATIVE SOLUTION IS SATURATED OR SUPERSATURATED. COMPUTE COEFFICIEN
C**** FOR QUADRATIC EQUATION
   40 CA(1) = 1.0
      CA(2) = SLCA + SLSO4
      CA(3) = (SLCA * SLSO4) - (2.4E-5 / GSQR)
      MOLE = 6RGYPSUM
CONVERT GYPSUM (SOLID) FROM MOLS/GRAM TO MOLES PER LITER - PRATIO IS
C**** MOISTURE CONTENT IN PERCENCT - MOLS/LITER = (1.0 /PRATIO)* 1.E5
      GYPSOL = GYPSUM * (1.0 /PRATIO) * 1.E5
      X = ROOTWO (KNODE,KSEG,CA, MOLE, IW)
      IF(X.LT.0.0)  GO TO 60
CONDITION-SOLUTION IS UNDERSATURED
      Y = GYPSOL - X
      IF(Y.LE.0.0)  GO TO 50
CONDITION - ENOUGH GYPSUM IN SOLID STATE TO SATURATE SOLUTION - UPDATE
C**** CALCIUM AND SULFATE   CONCENTRATIONS.
      SLCA = SLCA + X
      SLSO4 = SLSO4 + X
      GYPSOL = Y
      GO TO 70
CONDITION-NOT ENOUGH GYPSUM IN SOLID STATE TO SATURATE SOLUTION DISSOLVE
C**** ALL GYPSUM - UPDATE CALCIUM AND SULFATE CONCENTRATIONS
   50 GYPSOL = 0.0
      SLCA = SLCA + X
      SLSO4 = SLSO4 + X
      GO TO 100
CONDITION-SOLUTION IS SUPERSATURATED ADD EXCESS TO GYPSUM IN SOLID STATE
C**** UPDATE CALCIUM AND SULFATE CONCENTRATIONS
   60 X = ABS(X)
      GYPSOL = GYPSOL + X
      SLCA = SLCA - X
      SLSO4 = SLSO4 - X
CONDITION - TEST IF UNDISSOCIATED CASO4 (UCASO4) IS AT MAXIMUM CONCENTRATI
C**** OF 4.987E-3 MOLS /LITER
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      SUBROUTINE GYPEX (KNODE, KSEG, IW, PRATIO )

CONDITION - UCASO4 NOT AT MAXIMUM CONCENTRATION
      W = 4.987E-3 - UCASO4
      IF (W.LT.GYPSOL)  GO TO 80
CONDITION-NOT ENOUGH RESIDUAL GYPSUM TO BRING UCASO4 TO MAXIMUM CONCENTRAT
      UCASO4 = UCASO4 + GYPSOL
      GYPSOL = 0.0
      GO TO 100
CONDITION - ENOUGH RESIDUAL GYPSUM TO MEET MAXIMUM CONCENTRATION OF UCASO4
   80 GYPSOL = GYPSOL - W
      UCASO4 = 4.987E-3
CONVERT-RESIDUAL GYPSUM FOR MOLS/LITER BACK TO MOLS/GRAM
   90 GYPSUM = GYPSOL *  PRATIO / 1.E5
      GO TO 200
CALCULATE CHANGES IN CALCIUM AND SULFATE CONCENTRATIONS (X) TO SATISFY
C**** UNDISSOCIATED CASO4 (UCASO4) - WHERE EQUATION OF EQUILIBRIUM IS
C**** (UCASO4 -X ) K = GAMMA2**2((SLCA +X )(SLSO4 +X)) AND K = THERMODYNAM
C**** EQUILIBRIUM CONSTANT = 4.9E-3 - COEFFICIENTS FOR SECOND DEGREE
C**** EQUATION ARE AFTER RECOMPUTING IONIC STRENGTH
  100 GAMMA2 = GAMMA (2)
      GSQR = GAMMA2 * GAMMA2
  110 CA(1) = GSQR
      CA(2) = GSQR * (SLCA + SLSO4) + 4.9E-3
      CA(3) =(GSQR * SLCA* SLSO4) -(4.9E-3 * UCASO4)
      MOLE = 6RUCASO4
      X = ROOTWO (KNODE, KSEG, CA, MOLE ,IW)
C**** UPDATE CONCENTRATIONS OF CASO4, CA AND SO4
      UCASO4 = UCASO4 - X
      SLCA = SLCA + X
      SLSO4 = SLSO4 + X
CALCULATE CHANGES IN MAGNESIUM AND SULFATE CONCENTRATIONS (X) TO SATISFY
C**** UNDISSOCIATED MGSO4 (UMGSO4)- WHERE EQUATION OF EQUILIBRIUM IS
C**** (UMGSO4 -X ) K = GAMMA2**2((SLMG +X )(SLSO4 +X)) AND K = THERMODYNAM
C**** EQUILIBRIUM CONSTANT = 5.9E-3 - COEFFICIENTS FOR SECOND DEGREE
C**** EQUATION ARE -
  200 CA(1) = GSQR
      CA(2) = GSQR * (SLMG + SLSO4) + 5.9E-3
      CA(3) = (GSQR * SLMG * SLSO4) -(5.9E-3 * UMGSO4)
      MOLE = 6RUMGSO4
      X = ROOTWO (KNODE, KSEG, CA, MOLE, IW)
C**** UPDATE CONCENTRATIONS OF MGSO4, MG AND SO4
      UMGSO4 = UMGSO4 - X
      SLMG = SLMG + X
      SLSO4 = SLSO4 + X
 2000 RETURN
      END
      SUBROUTINE EXCANA ( KNODE , KSEG , IW, PRATIO )

C**** THIS SUBROUTINE CALCULATES THE SODIUM (MONOVALENT) EXCHANGE WITH
C**** CALCIUM(DIVALENT).       THE GAPON EQUATION EXPRESSING THE
C**** RELATIONSHIP OF CALCIUM AND SODIUM IN TERMS OF CONCENTRATIONS
C**** WAS USED. LET (X) REPRESENT THE CHANGE IN CONCENTRATION OF THE
C**** DIVALENT ION IN THE SOLID PHASE IN UNITS OF MOLS PER GRAM.
C**** CALCULATE COEFFICIENTS FOR THE FOURTH DEGREE POLYNOMIAL-- BETA
C**** IS THE CONVERSION FACTOR TO CONVERT MOLS PER GRAM TO MOLS
C**** PER LITER AND HAS UNITS OF GRAMS OF SOLID PER LITER OF SOLUTION
C**** EXCHANGE COEFFICIENT K (DEX) = 7.07E-1
      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                 SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLID/ CATEX, GYPSUM, SLIME ,RDENS, EXCA ,EXNA, EXMG ,
     1               EXTRAC , DEPTH, SEGVOL , INTER
      DIMENSION CA (10)
      DIMENSION T(4)
      DEX = 7.07E-1
C**** IF THERE IS NO SODIUM IN SOLUTION OR SOLID  PHASE EXIT ROUTINE
      IF ( SLNA .EQ. 0.0. AND.EXNA . EQ. 0.0 )  GO TO 2000
CALCULATE MONOVALENT ACTIVITY COEFFICIENT GAMMA1
      GAMMA1 = GAMMA (1)
      DO 50 K = 1, 10
      CA (K) = 0.0
   50 CONTINUE
      BETA = ( 1.0 / PRATIO) * 1.E5
C**** ARRANGE ORDER OF COEFFICIENTS IN INCREASING POWERS OF (X)
      GSQR = GAMMA1 * GAMMA1
      BETA2 = BETA * BETA
      DEX2 = DEX * DEX
      CA(1) = ( GSQR * EXNA * EXNA * SLCA ) - ( DEX2 * EXCA * EXCA
     1        * SLNA * SLNA )
      CA(2) = GSQR * EXNA * ( 4.0 * SLCA + BETA * EXNA ) + 2.0 * DEX2*
     1        EXCA * SLNA * ( SLNA + 2.0 * BETA * EXCA )
      CA(3) = 4.0 * GSQR * ( SLCA + BETA * EXNA ) - 4.0 * DEX2* BETA *
     1       EXCA * ( BETA * EXCA + 2.0 * SLNA ) - DEX2 * SLNA* SLNA
      CA(4) = 4.0 * BETA * ( 2.0 * DEX2 * EXCA * BETA + GSQR + DEX2 *
     1        SLNA )
      CA(5) = - 4.0*BETA2 * DEX2
      ISW = 1
CALCULATE A POSITIVE ROOT (REAL) IN RANGE XMIN - XMAX
      XMIN = 0.0
      XMAX = EXCA
      IF ( EXCA .GT. EXNA ) XMAX = EXNA
   60 MOLE = 6REXCANA
C**** SET CONVERGENCE CRITERION (TESTA) SO THAT F(X) IS LESS THAN 1.E-8
      TESTA = 1.E-8
      X = ROOT ( CONST, XMAX , XMIN , MOLE , CA , TESTA )
      IF ( MOLE . EQ . 5RTRUE  )  GO TO 68
      GO TO ( 75, 68 ) , ISW
C**** TEST ROOT TO INSURE NO UPDATED CONCENTRATIONS ARE LESS THAN ZERO
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      SUBROUTINE EXCANA ( KNODE , KSEG , IW, PRATIO )

      T(2) = EXCA - X
      T(3) = SLNA - ( 2.0 * BETA * X )
      T(4) = SLCA + ( BETA * X )
      DO 70 K = 1,4
      IF ( T (K) . LE.0.0 ) GO TO 75
   70 CONTINUE
      GO TO 80
   75 IF ( ISW . EQ. 2 )  GO TO 1000
CALCULATE A NEGATIVE ROOT (REAL) IN RANGE XMIN - XMAX
      XMIN = - XMAX
      XMAX= 0.0
      ISW = 2
      GO TO 60
C**** UPDATE CALCIUM AND SODIUM CONCENTRATIONS IN SOLUTION AND SOLID
C**** PHASES
   80 EXNA = T(1)
      EXCA = T(2)
      SLNA = T(3)
      SLCA = T(4)
      GO TO 2000
 1000 WRITE ( IW , 1005 ) KNODE , KSEG
 1005 FORMAT ( 1H1, 42HNO REAL ROOT EXISTS IN RANGE FOR CA-NA FOR  /
     1               7HNODE =    , I3 , 5X, 10HSEGMENT =    , I3 )
       WRITE ( IW, 1010 ) X, XMIN, XMAX, MOLE
 1010 FORMAT ( // 8X, 4HX = , F20.8 , 3X, 7HXMIN = , F20.8 , 3X,
     1                     7HXMAX = , F20.8, 3X, 7HMOLE =  , F5 )
      CALL EXIT
 2000 RETURN
      END
      SUBROUTINE EXCAMG ( KNODE, KSEG, IW, PRATIO )

      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                 SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLID/ CATEX, GYPSUM, SLIME ,BDENS, EXCA ,EXNA, EXMG ,
     1                EXTRAC , DEPTH, SEGVOL , INTER
C**** THIS SUBROUTINE CALCULATES THE MAGNESIUM (DIVALENT) EXCHANGE WITH
C**** CALCIUM (DIVALENT) . THE COMMON EQUATION EXPRESSING THE RELATIONSHIP
C**** OF CALCIUM AND MAGNESIUM IN TERMS OF CONCENTRATIONS WAS USED.
C**** LET (X) REPRESENT THE CHANGE IN CONCENTRATION OF THE DIVALENT ION
C**** IN THE SOLID PHASE IN UNITS OF MOLS PER GRAM. CALCULATE THE
C**** COEFFICIENTS OF SECOND DEGREE POLYNOMIAL - BETA = CONVERSION
C**** FACTOR TO CONVERT MOLS PER GRAM TO MOLS PER LITER AND HAS UNITS OF
C**** GRAMS OF SOLID PER LITER OF SOLUTION. EXCHANGE COEFFICIENT
C**** K (DEX) = 6.7E-1
      DIMENSION CA (10)
      DEX = 6.7E-1
      BETA = ( 1.0 / PRATIO ) * 1.E5
      CA(1) = BETA * ( 1.0 - DEX)
      CA(2)=BETA * ( DEX * EXCA + EXMG ) + DEX * SLMG + SLCA
      CA(3) = SLCA * EXMG - ( DEX * SLMG * EXCA )
      MOLE = 6RCALMAG
      X = ROOTWO ( KNODE , KSEG , CA , MOLE , IW )
C**** UPDATE CONCENTRATIONS OF CALCIUM AND MAGNESIUM IN SOLUTION AND
C**** SOLID PHASES
      SLCA = SLCA + ( BETA * X )
      SLMG = SLMG - ( BETA * X )
      EXCA = EXCA - X
      EXMG = EXMG + X
 2000 RETURN
      END
      SUBROUTINE CALCAR ( KNODE, KSEG, IN, PRATIO )

C**** THIS SUBROUTINE IS USED TO CALCULATE THE REACTION OF CALCIUM
C**** WITH THE CARBONATES. IF   CACO3 ( LIME ) IS PRESENT IN THE SOLID
C**** PHASE THE INDICATOR SLIME WILL BE SET TO ONE , IF LIME IS NOT
C**** PRESENT SLIME WILL BE SET TO ZERO . LOG10 (KPRIME )= -1.68 *
C**** LOG10 (PRATIO) - LOG10 (INTER) , WHERE PRATIO = MOISTURE CONTENT
C**** IN PERCENT, KPRIME = SLCA * SLHCO3 * SLHCO3 * GAMMA1 * GAMMA1
C**** * GAMMA2 AND INTER = INTERCEPT. THE EXPRESSION FOR KPRIME WAS
C**** DERIVED USING A SIMPLE LINEAR REGRESSION ( BY DUTT ET AL )
C**** WITH A LOGARITHMIC TRANSFORM.
      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                 SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLID/ CATEX, GYPSUM, SLIME ,BDENS, EXCA ,EXNA, EXMG ,
     1               EXTRAC , DEPTH, SEGVOL , INTER
      DIMENSION CA (10)
      REAL KPRIME , INTER
CHECK IF LIME IS PRESENT IN SOLID PHASE
      IF ( SLIME .EQ. 0.0 )  GO TO 50
C**** LIME IS PRESENT CALCULATE KPRIME
      IF (INTER . NE . 0.0 )  GO TO 43
   40 GAMMA1 = GAMMA (1)
      GAMMA2 = GAMMA (2)
      KPRIME = SLCA * SLHCO3 *SLHCO3 * GAMMA1 * GAMMA1 * GAMMA 2
COMPUTE INTERCEPT ONCE ONLY FOR EACH SOIL SEGMENT
      INTER = KPRIME * (PRATIO * * 1.68)
   43 KPRIME = INTER / (PRATIO ** 1.68 )
      DO 45 K = 1,10
      CA (K) = 0.0
   45 CONTINUE
      GO TO 55
C**** LIME IS NOT PRESENT IN SOLID PHASE ASSUME INTER = 4.52E2
   50 INTER = 4.52E2
      KPRIME = INTER / ( PRATIO ** 1.68)
      GO TO 100
CALCULATE SOLUBILITY OF  LIME ( CACO3) , USE EXPRESSION K = SLCA
C**** *SLHCO3*   SLHCO3 ** 2 * GAMMA1 **2 / SLH2CO3 ( THEN LET KPRIME
C**** = K * SLH2CO3.  LET (X) = CHANGE IN CONCENTRATION OF CALCIUM
C**** (DIVALENT)ION IN SOLUTION PHASE IN MOLS PER LITER. CALCULATE
C**** COEFFICIENTS FOR THIRD DEGREE POLYNOMIAL IN INCREASING POWERS  OF (X
CALCULATE A POSITIVE ROOT (REAL) IN RANGE XMIN - XMAX
   55 XMIN = 0.0
      XMAX = SLHCO3
      IF ( SLHCO3 . GT. SLCA ) XMAX = SLCA
      ISW = 1
   60 CA (1) = - KPRIME / ( GAMMA1 * GAMMA1 * GAMMA2 )
      CA (2) = 4.0 * SLCA * SLHCO3 + ( SLHCO3 * SLHCO3 )
      CA (3) = 4.0 * ( SLHCO3 + SLCA )
      CA (4) = 4.0
   65 MOLE = 6RCALCAR
      CONST = 0.0
      SUBROUTINE CALCAR ( KNODE, KSEG, IW, PRATIO )

      TESTA = 1.E-6
      X = ROOT ( CONST , XMAX , XMIN , MOLE , CA , TESTA )
      GO TO ( 67, 68 ) , ISW
   67 IF ( MOLE .EQ. 5RTRUE  ) GO TO 69
CALCULATE A NEGATIVE ROOT (REAL) IN RANGE XMIN - XMAX
      XMAX = 0.0
      XMIN = - XMAX
      ISW = 2
      GO TO 60
   68 IF ( MOLE .NE. 5RTRUE  ) GO TO 1000
C**** UPDATE CONCENTRATIONS OF CALCIUM (SLCA) AND BICARBONATE (SLHCO3)
C**** IN SOLUTION
   69 SLCA = SLCA + X
      SLHCO3 = SLHCO3 + X
   70 IF (SLIME . GT. 0.0 ) GO TO 2000
  100 TEMP = SLCA * SLHCO3 * SLHCO3 * GAMMA1 * GAMMA1 * GAMMA2
      IF ( TEMP .GE. KPRIME )  GO TO 43
      GO TO 2000
 1000 WRITE ( IW, 1005 ) KNODE , KSEG
 1005 FORMAT(1H1, 8X, 28HNO REAL ROOT FOUND IN CALCAR  / 8X,
     1              7HNODE =     , I3 , 5X, 10HSEGMENT =  , I3 )
      CALL EXIT
 2000 RETURN
      END
      SUBROUTINE SCRIBE (IW)

      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                   SLNO3 ,UCASO4 , UMGSO4
      COMMON /SOLID/ CATEX, GYPSUM, SLIME ,BDENS, EXCA ,EXNA, EXMG ,
     1                 EXTRAC , DEPTH, SEGVOL  , INTER
      REAL INTER
      WRITE ( IW , 10 ) SLCA, SLMG, SLNA, SLCL , SLSO4 , SLHCO3 , SLNO3,
     1       SLCO3,       EXTRAC, SEGVOL, CATEX, GYPSUM, SLIME , BDENS,
     2                    DEPTH , EXCA, EXNA, EXMG, UCASO4 , UMGSO4  ,
     3                    INTER
   10 FORMAT (        8X, 9HSLCA     =  , F20.8/
     1                8X, 9HSLMG     =  , F20.8/
     1                8X, 9HSLNA     =  , F20.8/
     1                8X, 9HSLCL     =  , F20.8/
     1                8X, 9HSLSO4    =  , F20.8/
     1                8X, 9HSLHCO3   =  , F20.8/
     1                8X, 9HSLNO3    =  , F20.8/
     1                8X, 9HSLCO3    =  , F20.8/
     1                8X, 9HEXTRAC   =  , F20.8/
     1                8X, 9HSEGVOL   =  , F20.8/
     1                8X, 9HCATEX    =  , F20.8/
     1                8X, 9HGYPSUM   =  , F20.8/
     1                8X, 9HSLIME    =  , F20.8/
     1                8X, 9HBDENS    =  , F20.8/
     1                8X, 9HDEPTH    =  , F20.8/
     1                8X, 9HEXCA     =  , F20.8/
     1                8X, 9HEXNA     =  , F20.8/
     1                8X, 9HEXMG     =  , F20.8/
     1                8X, 9HUCASO4   =  , F20.8/
     1                8X, 9HUMGSO4   =  , F20.8/
     1                8X, 9HINTER    =  , F20.8/
       RETURN
       END
      FUNCTION GAMMA ( KVAL )

C*****
C**** THIS FUNCTION CALCULATES THE ACTIVITY COEFFICIENT (GAMMA)
C**** FOR MONOVALFNT ION ( KVAL = 1) AND DIVALENT ION ( KVAL = 2 )
C*****
      COMMON /SOLUTE / SLCA, SLMG, SLNA, SLCL , SLSO4, SLHCO3, SLCO3,
     1                 SLNO3 ,UCASO4 , UMGSO4
CALCULATE THE IONIC STRENGTH OF ALL SPECIES IN SOLUTION (U) WHERE
C**** U= 1/2 (SUMMATION OF CONCENTRATION OF ION ( MOLS/LITFR) TIMES
C**** VALENCE OF ION SQUARED - FOR ALL SPECIES)
      U = 2.0 * (SLCA + SLMG + SLSO4 + SLCO3) + 5.E-1 * (SLNA + SLCL +
     1    SLNO3 + SLHCO3 )
CALCULATE ACTIVITY COEFFICIENT ******************** ION USING DEBYE-
C**** HUCKEL FORMULA AS A FUNCTION OF IONIC STRENGTH AND VALENCE
      COMP = 0.0
      COMP = SQRT(U)
      GO TO ( 50, 100) , KVAL
   50 GAMMA = EXP ( -1.17201 * COMP / ( 1.0 + COMP ))
      GO TO 200
  100 GAMMA = EXP ( -4.68804 * COMP / ( 1.0 + COMP ))
  200 RETURN
      END
```